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(FILE 'HOME' ENTERED AT 09:15:43 ON 05 SEP 2006)  
FILE 'BIOSIS' ENTERED AT 09:15:53 ON 05 SEP 2006  
FILE 'REGISTRY' ENTERED AT 09:16:13 ON 05 SEP 2006  
E "LEVOTHYROXINE"/CN 25  
L1 2 S E3 OR E4  
E "LEVOTHYROXINE"/CN 25  
E "LIOTHRONINE"/CN 25  
E "TRIIODOTHYRONINE"/CN 25  
L2 9 S E3 OR E12 OR E13 OR E14 OR E15 OR E16 OR E19 OR E20 OR E21 OR  
E "DIIODOTHYRONINE"/CN 25  
L3 1 S E3  
FILE 'HOME' ENTERED AT 09:23:41 ON 05 SEP 2006  
FILE 'HCAPLUS' ENTERED AT 09:38:19 ON 05 SEP 2006  
E "55-03-8"/BI,RN 25  
L4 481 S E3 OR E5  
L5 9 S L4 AND ETHANOL  
E "64-17-5"/BI,RN 25  
L6 197111 S E3  
L7 6 S L6 AND L4  
L8 4 S L5 AND 1800<=PY<=1995  
E DICKINSON J/AU 25  
E DICKINSON JEFFREY/AU 25  
L9 1 S (E3) AND (THYROID OR THYRONINE OR LEVOTHYROXINE OR TETRAIODOT  
E KHAN KARRAR/AU 25  
L10 3 S (E3 OR E4 OR E5 OR E6) AND (THYROID OR THYRONINE OR LEVOTHYRO  
E HAGUE JOHN/AU 25  
L11 1 S (E4 OR E7 OR E8) AND (THYROID OR THYRONINE OR LEVOTHYROXINE O  
E SMITH ALAN/AU 25  
L12 3 S (E3) AND (THYROID OR THYRONINE OR LEVOTHYROXINE OR TETRAIODOT  
FILE 'HOME' ENTERED AT 09:50:33 ON 05 SEP 2006  
FILE 'REGISTRY' ENTERED AT 10:00:41 ON 05 SEP 2006  
L13 1 S 5817-39-0/RN  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY  
FILE 'REGISTRY' ENTERED AT 10:01:52 ON 05 SEP 2006  
L14 1 S 6893-02-3/RN  
SET NOTICE 1 DISPLAY  
SET NOTICE LOGIN DISPLAY  
FILE 'HOME' ENTERED AT 10:02:48 ON 05 SEP 2006

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'BIOSIS' ENTERED AT 09:15:53 ON 05 SEP 2006  
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FILE COVERS 1969 TO DATE.  
 CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT  
 FROM JANUARY 1969 TO DATE.

RECORDS LAST ADDED: 30 August 2006 (20060830/ED)

=> FIL REGISTRY	SINCE FILE ENTRY	TOTAL SESSION
COST IN U.S. DOLLARS		
FULL ESTIMATED COST	0.87	1.08

FILE 'REGISTRY' ENTERED AT 09:16:13 ON 05 SEP 2006  
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STRUCTURE FILE UPDATES: 4 SEP 2006 HIGHEST RN 905816-92-4  
 DICTIONARY FILE UPDATES: 4 SEP 2006 HIGHEST RN 905816-92-4

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when  
 conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
 predicted properties as well as tags indicating availability of  
 experimental property data in the original document. For information  
 on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> E "LEVOTHYROXINE"/CN 25	
E1	1 LEVOTHYM/CN
E2	1 LEVOTHYROX/CN
E3	1 ---> LEVOTHYROXINE/CN
E4	1 LEVOTHYROXINE SODIUM/CN
E5	1 LEVOTININE/CN
E6	1 LEVOTIROX/CN
E7	1 LEVOTIROXINA/CN
E8	1 LEVOTOFISOPAM/CN
E9	1 LEVOTOMIN/CN
E10	1 LEVOVERMAX/CN
E11	1 LEVOVETIN/CN
E12	1 LEVOVIRIN/CN
E13	1 LEVOVIST/CN
E14	1 LEVOXADROL/CN
E15	1 LEVOXADROL HYDROCHLORIDE/CN
E16	1 LEVOXAN/CN
E17	1 LEVOXIN 15/CN
E18	1 LEVOXINE/CN
E19	1 LEVOXYL/CN
E20	1 LEVR (BACILLUS LICHENIFORMIS STRAIN DSM13 GENE LEVR) /CN

E21 1 LEVRAZOXANE/CN  
 E22 1 LEVSIN/CN  
 E23 1 LEVSIN SULFATE/CN  
 E24 1 LEVSINEX/CN  
 E25 1 LEVSPHERE 100G/CN

=> S E3 OR E4

1 LEVOTHYROXINE/CN  
 1 "LEVOTHYROXINE SODIUM"/CN  
 L1 2 LEVOTHYROXINE/CN OR "LEVOTHYROXINE SODIUM"/CN

=> DIS L1 1 RN CCN

THE ESTIMATED COST FOR THIS REQUEST IS 1.90 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L1 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2006 ACS on STN

RN 55-03-8 REGISTRY

CN L-Tyrosine, O-(4-hydroxy-3,5-diiodophenyl)-3,5-diido-, monosodium salt  
 (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Thyroxine, monosodium salt, L- (8CI)

OTHER NAMES:

CN Berlthyrox; Dathroid; Droxine; Eferox; Elthyrone; Elthyroxine;  
 Eltroxin; Euthyrox; Eutirox; L-Thyroxin Henning; L-Thyroxine  
 monosodium salt; L-Thyroxine sodium; L-Thyroxine sodium salt; Laevoxin;  
 Letrox; Letter; Levaxin; Levo-T; Levoroxine; Levothroid; Levothyrox;  
 Levothyroxine sodium; Levotirox; Levotiroxina; Levoxyl;  
 Monosodium thyroxine; NSC 259940; Oroxine; Puran T 4; Sodium  
 L-thyroxine; Sodium levothyroxine; Sodium thyroxin; Sodium thyroxinate;  
 Sodium thyroxine; Synthroid; Synthroid sodium; Synthrox; T 4KP;  
 Thevier; Throxinique; Thyradin; Thyradin S; Thyrax Duotab; Thyrex;  
 Thryo 4; Thyrosit; Thyroxevan; Thyroxine sodium; Thyroxine sodium  
 salt; Tirodine

=> E "LEVOTHYROXINE"/CN 25

E1 1 LEVOTHYM/CN  
 E2 1 LEVOTHYROX/CN  
 E3 1 --> LEVOTHYROXINE/CN  
 E4 1 LEVOTHYROXINE SODIUM/CN  
 E5 1 LEVOTININE/CN  
 E6 1 LEVOTIROX/CN  
 E7 1 LEVOTIROXINA/CN  
 E8 1 LEVOTOFISOPAM/CN  
 E9 1 LEVOTOMIN/CN  
 E10 1 LEVOVERMAX/CN  
 E11 1 LEVOVETIN/CN  
 E12 1 LEVOVIRIN/CN  
 E13 1 LEVOVIST/CN  
 E14 1 LEVOXADROL/CN  
 E15 1 LEVOXADROL HYDROCHLORIDE/CN  
 E16 1 LEVOXAN/CN  
 E17 1 LEVOXIN 15/CN  
 E18 1 LEVOXINE/CN  
 E19 1 LEVOXYL/CN  
 E20 1 LEVR (BACILLUS LICHENIFORMIS STRAIN DSM13 GENE LEVR) /CN  
 E21 1 LEVRAZOXANE/CN  
 E22 1 LEVSIN/CN  
 E23 1 LEVSIN SULFATE/CN  
 E24 1 LEVSINEX/CN  
 E25 1 LEVSPHERE 100G/CN

=> E "LIOTHRONINE"/CN 25

E1 1 LIOTHENE G 4116, POLYMER WITH 1,2-BENZENEDICARBOXYLIC ACID,  
 1,4-BUTANEDIOL, 2-ETHYL-2-(HYDROXYMETHYL)-1,3-PROPANEDIOL AND HEXANEDIOIC ACID/CN

E2 1 LIOTHENE M 1063-4/CN  
 E3 0 --> LIOTHRONINE/CN  
 E4 1 LIOTHYRONIINDE SODIUM SALT/CN  
 E5 1 LIOTHYRONIN/CN  
 E6 1 LIOTHYRONIN SODIUM/CN  
 E7 1 LIOTHYRONINE/CN  
 E8 1 LIOTHYRONINE HYDROCHLORIDE/CN  
 E9 1 LIOTHYRONINE I-125/CN  
 E10 1 LIOTHYRONINE I-131/CN  
 E11 1 LIOTHYRONINE SODIUM/CN  
 E12 1 LIOTON 1000/CN  
 E13 1 LIOTRAN SS/CN  
 E14 1 LIOTRIX/CN  
 E15 1 LIOTRON UR 4532/CN  
 E16 1 LIOTRON UR 4599-22/CN  
 E17 1 LIOTRON UR 4619/CN  
 E18 1 LIOTTITE/CN  
 E19 1 LIOURETHANE JRU 140/CN  
 E20 1 LIOUVILLOSIDE A/CN  
 E21 1 LIOUVILLOSIDE B/CN  
 E22 1 LIOVAC 3016/CN  
 E23 1 LIOVAC 3024/CN  
 E24 1 LIOVAC 3043/CN  
 E25 1 LIOVIL/CN

=> E "TRIIODOTHYRONINE"/CN 25

E1 1 TRIIODOTETRAKIS (THF) URANIUM/CN  
 E2 1 TRIIODOTHYROFORMIC ACID/CN  
 E3 1 --> TRIIODOTHYRONINE/CN  
 E4 1 TRIIODOTHYRONINE 5'-MONODEIODINASE/CN  
 E5 1 TRIIODOTHYRONINE 5-DEIODINASE/CN  
 E6 1 TRIIODOTHYRONINE 5-DEIODINASE (SUS SCROFA) /CN  
 E7 1 TRIIODOTHYRONINE 5-MONODEIODINASE/CN  
 E8 1 TRIIODOTHYRONINE AMINOTRANSFERASE/CN  
 E9 1 TRIIODOTHYRONINE DEIODINASE/CN  
 E10 1 TRIIODOTHYRONINE GLUCURONIDE/CN  
 E11 1 TRIIODOTHYRONINE GLUCURONOSYLTRANSFERASE/CN  
 E12 1 TRIIODOTHYRONINE HYDROCHLORIDE/CN  
 E13 1 TRIIODOTHYRONINE LABELED WITH IODINE-125/CN  
 E14 1 TRIIODOTHYRONINE LABELED WITH IODINE-131/CN  
 E15 1 TRIIODOTHYRONINE MAGNESIUM SALT/CN  
 E16 1 TRIIODOTHYRONINE POTASSIUM SALT/CN  
 E17 1 TRIIODOTHYRONINE RECEPTOR (HUMAN GENE THRA1) /CN  
 E18 1 TRIIODOTHYRONINE RECEPTOR (HUMAN) /CN  
 E19 1 TRIIODOTHYRONINE SODIUM SALT/CN  
 E20 1 TRIIODOTHYRONINE SULFAMATE/CN  
 E21 1 TRIIODOTHYRONINE SULFATE/CN  
 E22 1 TRIIODOTHYRONINE SULFOTRANSFERASE/CN  
 E23 1 TRIIODOTHYRONINE SULFOTRANSFERASE (HUMAN LIVER GENE ST1B2) /CN  
 E24 1 TRIIODOTHYRONINE SULFOTRANSFERASE (RAT LIVER GENE ST1B1) /CN  
 E25 1 TRIIODOTHYRONINE-131I/CN

=> S E3 OR E12 OR E13 OR E14 OR E15 OR E16 OR E19 OR E20 OR E21 OR E25

1 TRIIODOTHYRONINE/CN  
 1 "TRIIODOTHYRONINE HYDROCHLORIDE"/CN  
 1 "TRIIODOTHYRONINE LABELED WITH IODINE-125"/CN  
 1 "TRIIODOTHYRONINE LABELED WITH IODINE-131"/CN  
 1 "TRIIODOTHYRONINE MAGNESIUM SALT"/CN  
 1 "TRIIODOTHYRONINE POTASSIUM SALT"/CN  
 1 "TRIIODOTHYRONINE SODIUM SALT"/CN  
 1 "TRIIODOTHYRONINE SULFAMATE"/CN  
 1 "TRIIODOTHYRONINE SULFATE"/CN  
 1 TRIIODOTHYRONINE-131I/CN

L2 9 TRIIODOTHYRONINE/CN OR "TRIIODOTHYRONINE HYDROCHLORIDE"/CN OR  
 "TRIIODOTHYRONINE LABELED WITH IODINE-125"/CN OR "TRIIODOTHYRONINE LABELED WITH  
 IODINE-131"/CN OR "TRIIODOTHYRONINE MAGNESIUM SALT"/CN OR "TRIIODOTHYRONINE POTASSIUM SALT"/

CN OR "TRIIODOTHYRONINE SODIUM SALT"/CN OR "TRIIODOTHYRONINE SULFAMATE"/CN OR "TRIIODOTHYRONINE SULFATE"/CN OR TRIIODOTHYRONINE-131I/CN

=> DIS L2 1 RN CCN

THE ESTIMATED COST FOR THIS REQUEST IS 1.90 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L2 ANSWER 1 OF 9 REGISTRY COPYRIGHT 2006 ACS on STN

RN 892548-39-9 REGISTRY

CN L-Tyrosine, O-(4-hydroxy-3-iodophenyl)-3,5-diiodo-, monopotassium salt (9CI) (CA INDEX NAME)

OTHER NAMES:

CN Triiodothyronine potassium salt

=> E "DIIODOTHYRONINE"/CN 25

E1 1 DIIODOTHIOCYANATOORTHOSULFUROUS ACID/CN

E2 1 DIODOTHYMOL/CN

E3 1 --> DIIODOTHYRONINE/CN

E4 1 DIIODOTHYRONINE SULFOTRANSFERASE/CN

E5 1 DIODOTHYROTROPIN-RELEASING FACTOR/CN

E6 1 DIODOTIN/CN

E7 1 DIODOTIN PHTHALOCYANINE/CN

E8 1 DIODOTIN(1+)/CN

E9 1 DIODOTITANIUM/CN

E10 1 DIODOTITANOCENE/CN

E11 1 DIODOTOLUENE/CN

E12 1 DIODOTOLYLBORANE/CN

E13 1 DIODOTRIBUTYLPHOSPHORANE/CN

E14 1 DIODOTRIISOPROPYLARSENIC/CN

E15 1 DIODOTRIMETHYL ANTIMONY/CN

E16 1 DIODOTRIMETHYLARSENIC/CN

E17 1 DIODOTRIMETHYLARSORANE/CN

E18 1 DIODOTRIMETHYLPHOSPHORANE/CN

E19 1 DIODOTRIPHENYLANTIMONY/CN

E20 1 DIODOTRIPHENYLPHOSPHORANE/CN

E21 1 DIODOTRIPOXYLPHOSPHORANE/CN

E22 1 DIODOTRIS (M-METHYLPHENYL) PHOSPHORANE/CN

E23 1 DIODOTRIS (P-(METHYLTHIO) PHENYL) PHOSPHORANE/CN

E24 1 DIODOTRIS (P-METHOXYPHENYL) PHOSPHORANE/CN

E25 1 DIODOTRIS (TETRAHYDROFURAN) DYSPROSIUM/CN

=> S E3

L3 1 DIODOTHYRONINE/CN

=> DIS L3 1 RN CCN

THE ESTIMATED COST FOR THIS REQUEST IS 1.90 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 1041-01-6 REGISTRY

CN L-Tyrosine, O-(4-hydroxyphenyl)-3,5-diiodo- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Alanine, 3-[4-(p-hydroxyphenoxy)-3,5-diiodophenyl]-, L- (8CI)

OTHER NAMES:

CN 3,5-Diido-L-thyronine; 3,5-Diiodothyronine; Diido-L-thyronine; Diiodothyronine; L-3,5-Diiodothyronine; L-Diiodothyronine; L-T2; NSC 90469; O-(4-Hydroxyphenyl)-3,5-diido-L-tyrosine

=> DIS L3 1 FIDE

THE ESTIMATED COST FOR THIS REQUEST IS 4.68 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

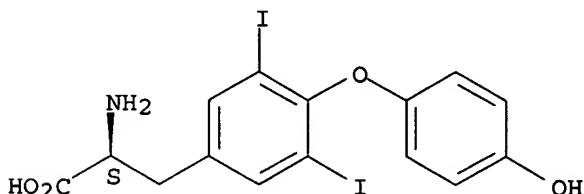
L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 1041-01-6 REGISTRY  
 ED Entered STN: 16 Nov 1984  
 CN L-Tyrosine, O-(4-hydroxyphenyl)-3,5-diiodo- (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN Alanine, 3-[4-(p-hydroxyphenoxy)-3,5-diiodophenyl]-, L- (8CI)  
 OTHER NAMES:  
 CN 3,5-Diiodo-L-thyronine  
 CN 3,5-Diiodothyronine  
 CN Diiodo-L-thyronine  
 CN Diiodothyronine  
 CN L-3,5-Diiodothyronine  
 CN L-Diiodothyronine  
 CN L-T2  
 CN NSC 90469  
 CN O-(4-Hydroxyphenyl)-3,5-diiodo-L-tyrosine  
 FS STEREOSEARCH  
 DR 30804-67-2, 243965-18-6  
 MF C15 H13 I2 N O4  
 CI COM  
 LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN\*, BIOSIS, BIOTECHNO, CA, CAOLD,  
     CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CSCHEM, EMBASE, GMELIN\*, IPA, PS,  
     TOXCENTER, USPAT2, USPATFULL  
     (\*File contains numerically searchable property data)  
 Other Sources: EINECS\*\*  
     (\*\*Enter CHEMLIST File for up-to-date regulatory information)  
 DT.CA CAplus document type: Conference; Journal; Patent; Report  
 RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);  
     PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES  
     (Uses); NORL (No role in record)  
 RLD.P Roles for non-specific derivatives from patents: ANST (Analytical  
     study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP  
     (Properties); USES (Uses)  
 RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological  
     study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP  
     (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or  
     reagent); USES (Uses); NORL (No role in record)  
 RLD.NP Roles for non-specific derivatives from non-patents: BIOL (Biological  
     study); FORM (Formation, nonpreparative); PREP (Preparation); PRP  
     (Properties)

#### Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2

Absolute stereochemistry. Rotation (+).



#### Experimental Properties (EPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
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IR Absorption Spectra	Spectrum		(1)	AIST
Melting Point (MP)	256 deg C		(2)	CAS
Melting Point (MP)	253 deg C (decomp)		(3)	CAS
Optical Rotatory Power (ORP)	+24.9 deg	Temp: 21 deg C Wavlen: 589.3 nm	(3)	CAS
Optical Rotatory Power (ORP)	-26 deg	Temp: 25 deg C Wavlen: 589.3 nm	(2)	CAS

(1) "Integrated Spectral Data Base System of Organic Compounds" data were obtained from the National Institute of Advanced Industrial Science and Technology (Japan)  
 (2) Meltzer, Robert I.; US 3102136 1963 CAPLUS  
 (3) Varcoe, J. S.; Journal of the Chemical Society 1960 P2711-15 CAPLUS

IR Absorption Spectra  
 / BINARY DATA / 659001.GIF  
 Spectrum ID: NIDA3807  
 Spectrometer: Nicolet 170SX or JASCO FT/IR-410  
 Source: "Integrated Spectral Data Base System of Organic Compounds" data were obtained from the National Institute of Advanced Industrial Science and Technology (Japan)

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Experimental Property Tags (ETAG)

PROPERTY	NOTE
Bond Angle	(1) CAS
IR Spectra	(1) CAS
Mass Spectra	(2) CAS
Raman Spectra	(1) CAS

(1) Alvarez, Rosa M. S.; Journal of Raman Spectroscopy 2004 V35(11) P947-955 CAPLUS  
 (2) Wang, Zongyi; Fenxi Huaxue 2003 V31(10) P1187-1190 CAPLUS

Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1.0	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	1.27	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	1.38	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	1.40	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	1.40	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	1.38	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	1.26	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 10 25 deg C	(1)
Boiling Point (BP)	559.4+/-50.0 deg C	760 Torr	(1)
Density (DEN)	2.095+/-0.06 g/cm**3	760 Torr	(1)
Enthalpy of Vap. (HVAP)	88.56+/-3.0 kJ/mol	760 Torr	(1)
Flash Point (FP)	292.1+/-30.1 deg C		(1)
Freely Rotatable Bonds (FRB)	7		(1)
H acceptors (HAC)	5		(1)
H donors (HD)	4		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	9		(1)
Koc (KOC)	2.59	pH 1 25 deg C	(1)
Koc (KOC)	4.84	pH 2 25 deg C	(1)

Koc (KOC)	7.82	pH 3 25 deg C	(1)
Koc (KOC)	8.52	pH 4 25 deg C	(1)
Koc (KOC)	8.60	pH 5 25 deg C	(1)
Koc (KOC)	8.60	pH 6 25 deg C	(1)
Koc (KOC)	8.52	pH 7 25 deg C	(1)
Koc (KOC)	7.74	pH 8 25 deg C	(1)
Koc (KOC)	3.92	pH 9 25 deg C	(1)
Koc (KOC)	1.0	pH 10 25 deg C	(1)
LOGD (LOGD)	0.76	pH 1 25 deg C	(1)
LOGD (LOGD)	1.03	pH 2 25 deg C	(1)
LOGD (LOGD)	1.24	pH 3 25 deg C	(1)
LOGD (LOGD)	1.28	pH 4 25 deg C	(1)
LOGD (LOGD)	1.28	pH 5 25 deg C	(1)
LOGD (LOGD)	1.28	pH 6 25 deg C	(1)
LOGD (LOGD)	1.28	pH 7 25 deg C	(1)
LOGD (LOGD)	1.24	pH 8 25 deg C	(1)
LOGD (LOGD)	0.94	pH 9 25 deg C	(1)
LOGD (LOGD)	0.07	pH 10 25 deg C	(1)
LOGP (LOGP)	3.782+-0.627	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	0.16 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	0.95 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.15 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.074 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.063 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.063 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.063 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.063 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.068 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.15 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	1.9 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.063 g/L	Unbuffered Water	(1)
		pH 6.41	
		25 deg C	
		25 deg C	(1)
Molar Intrinsic Solubility (ISLB.MOL)	0.00031 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0018 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00029 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00014 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00012 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00012 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00012 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00013 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00028 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0036 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00012 mol/L	Unbuffered Water	(1)
		pH 6.41	
		25 deg C	
		20 deg C	(1)
		760 Torr	
Molar Volume (MVOL)	250.5+-3.0 cm**3/mol	25 deg C	(1)
Molecular Weight (MW)	525.08	Most Acidic	(1)
PKA (PKA)	2.15+-0.30	25 deg C	(1)
PKA (PKA)	8.99+-0.45	Most Basic	(1)
Polar Surface Area (PSA)	92.78 A**2	25 deg C	(1)
Vapor Pressure (VP)	2.39E-13 Torr	25 deg C	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14  
 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.  
 419 REFERENCES IN FILE CA (1907 TO DATE)

15 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
419 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
9 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

START LOCAL KERMIT RECEIVE PROCESS

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(FILE 'HOME' ENTERED AT 09:15:43 ON 05 SEP 2006)

FILE 'BIOSIS' ENTERED AT 09:15:53 ON 05 SEP 2006

FILE 'REGISTRY' ENTERED AT 09:16:13 ON 05 SEP 2006

    E "LEVOTHYROXINE"/CN 25

L1      2 S E3 OR E4

    E "LEVOTHYROXINE"/CN 25

    E "LIOTHRONINE"/CN 25

    E "TRIIODOTHYRONINE"/CN 25

L2      9 S E3 OR E12 OR E13 OR E14 OR E15 OR E16 OR E19 OR E20 OR E21 OR

    E "DIIODOTHYRONINE"/CN 25

L3      1 S E3

=> DIS L1 1 FIDE

THE ESTIMATED COST FOR THIS REQUEST IS 4.68 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L1   ANSWER 1 OF 2 REGISTRY COPYRIGHT 2006 ACS on STN

RN   55-03-8 REGISTRY

ED   Entered STN: 16 Nov 1984

CN   L-Tyrosine, O-(4-hydroxy-3,5-diiodophenyl)-3,5-diido-, monosodium salt  
(9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN   Thyroxine, monosodium salt, L- (8CI)

OTHER NAMES:

CN   Berlthyrox

CN   Dathroid

CN   Droxine

CN   Eferox

CN   Elthyrone

CN   Elthyroxine

CN   Eltroxin

CN   Euthyrox

CN   Eutirox

CN   L-Thyroxin Henning

CN   L-Thyroxine monosodium salt

CN   L-Thyroxine sodium

CN   L-Thyroxine sodium salt

CN   Laevoxin

CN   Letrox

CN   Letter

CN   Levaxin

CN   Levo-T

CN   Levoroxine

CN   Levothroid

CN   Levothyrox

CN   Levothyroxine sodium

CN   Levotirox

CN   Levotiroxina

CN   Levoxyl

CN   Monosodium thyroxine

CN   NSC 259940

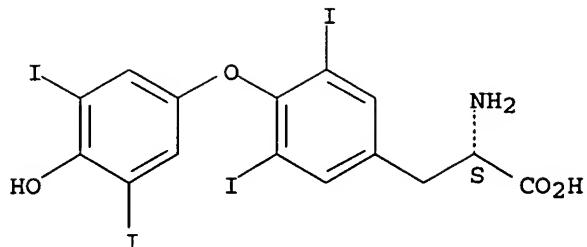
CN   Oroxine

CN Puran T 4  
 CN Sodium L-thyroxine  
 CN Sodium levothyroxine  
 CN Sodium thyroxin  
 CN Sodium thyroxinate  
 CN Sodium thyroxine  
 CN Synthroid  
 CN Synthroid sodium  
 CN Synthrox  
 CN T 4KP  
 CN Thevier  
 CN Throxinique  
 CN Thryadin  
 CN Thryadin S  
 CN Thryax Duotab  
 CN Thyrex  
 CN Thyro 4  
 CN Thyrosit  
 CN Thyroxevan  
 CN Thyroxine sodium  
 CN Thyroxine sodium salt  
 CN Tiroidine  
 FS STEREOSEARCH  
 DR 50809-32-0, 67809-22-7  
 MF C15 H11 I4 N O4 . Na  
 CI COM  
 LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN\*, BIOSIS,  
     BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMLIST, CIN,  
     CSCHEM, DDFU, DRUGU, EMBASE, IMSCOSEARCH, IPA, MEDLINE, MRCK\*, MSDS-OHS,  
     PIRA, PROMT, PS, RTECS\*, TOXCENTER, USAN, USPAT2, USPATFULL, VETU  
     (\*File contains numerically searchable property data)  
 Other Sources: EINECS\*\*, NDSL\*\*, TSCA\*\*, WHO  
     (\*\*Enter CHEMLIST File for up-to-date regulatory information)  
 DT.CA CAplus document type: Conference; Dissertation; Journal; Patent; Report  
 RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);  
     PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or  
     reagent); USES (Uses)  
 RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological  
     study); PREP (Preparation); PROC (Process); PRP (Properties); RACT  
     (Reactant or reagent); USES (Uses); NORL (No role in record)  
 CRN (51-48-9)

## Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2

Absolute stereochemistry.



● Na

#### Experimental Properties (EPROP)

PROPERTY (CODE)	VALUE	NOTE
IR Absorption Spectra	Spectrum	(1) AIST

(1) "Integrated Spectral Data Base System of Organic Compounds" data were obtained from the National Institute of Advanced Industrial Science and Technology (Japan)

IR Absorption Spectra  
 / BINARY DATA / 659002.GIF  
 Spectrum ID: NIDA73353  
 Spectrometer: Nicolet 170SX or JASCO FT/IR-410  
 Source: "Integrated Spectral Data Base System of Organic Compounds" data were obtained from the National Institute of Advanced Industrial Science and Technology (Japan)

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#### Experimental Property Tags (ETAG)

PROPERTY	NOTE
ADME (Absorption, Distribution, Metabolism, Excretion)	(1) CAS
IR Absorption Spectra	(2) CAS
Thermal Analysis	(2) CAS

(1) Walter-Sack, Ingeborg; Clinical Pharmacokinetics 2004 V43(14)  
 P1037-1053 CAPLUS  
 (2) Westenberger, Benjamin J.; International Journal of Pharmaceutics 2005  
 V306(1-2) P56-70 CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.

480 REFERENCES IN FILE CA (1907 TO DATE)  
 481 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

START LOCAL KERMIT RECEIVE PROCESS

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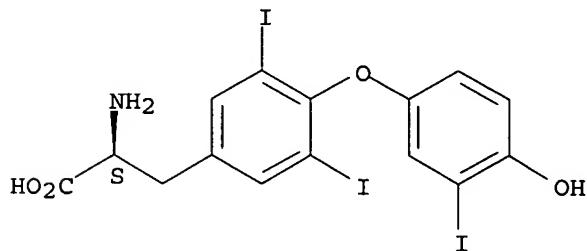
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 THE ESTIMATED COST FOR THIS REQUEST IS 4.68 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L2 ANSWER 1 OF 9 REGISTRY COPYRIGHT 2006 ACS on STN  
 RN 892548-39-9 REGISTRY  
 ED Entered STN: 14 Jul 2006  
 CN L-Tyrosine, O-(4-hydroxy-3-iodophenyl)-3,5-diiodo-, monopotassium salt  
 (9CI) (CA INDEX NAME)  
 OTHER NAMES:  
 CN Triiodothyronine potassium salt  
 FS STEREOSEARCH  
 MF C15 H12 I3 N O4 . K  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 DT.CA CAplus document type: Patent  
 RL.P Roles from patents: PREP (Preparation)  
 CRN (6893-02-3)

## Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence Count
EA	ES	SZ	RF	RID	
C6	C6	6	C6	46.150.18	2

Absolute stereochemistry. Rotation (+).



● K

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> FIL HOME  
 COST IN U.S. DOLLARS SINCE FILE TOTAL  
 ENTRY SESSION  
 FULL ESTIMATED COST 83.33 84.41

FILE 'HOME' ENTERED AT 09:23:41 ON 05 SEP 2006

=> FIL HCAPLUS  
 COST IN U.S. DOLLARS SINCE FILE TOTAL  
 ENTRY SESSION  
 FULL ESTIMATED COST 5.04 89.45

FILE 'HCAPLUS' ENTERED AT 09:38:19 ON 05 SEP 2006  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 5 Sep 2006 VOL 145 ISS 11  
 FILE LAST UPDATED: 4 Sep 2006 (20060904/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> E "55-03-8"/BI,RN 25  
 E1 1 55-01-6P/BI  
 E2 6 55-02-7/BI  
 E3 481 --> 55-03-8/BI  
 E4 0 55-03-8/RN  
 E5 4 55-03-8P/BI  
 E6 152 55-06-1/BI  
 E7 1 55-06-1D/BI  
 E8 1 55-06-1DP/BI  
 E9 3 55-06-1P/BI  
 E10 2 55-07-2/BI  
 E11 1 55-08-3/BI  
 E12 2 55-09-4/BI  
 E13 1 55-10-2/BI  
 E14 2123 55-10-7/BI  
 E15 16 55-10-7D/BI  
 E16 5 55-10-7DP/BI  
 E17 37 55-10-7P/BI  
 E18 7 55-11-8/BI  
 E19 2 55-11-8P/BI  
 E20 1 55-12-1/BI  
 E21 1 55-14-1/BI  
 E22 87 55-16-3/BI  
 E23 1 55-16-3D/BI  
 E24 3 55-16-3P/BI  
 E25 2 55-17-4/BI

=> S E3 OR E5  
 481 55-03-8/BI  
 4 55-03-8P/BI  
 L4 481 55-03-8/BI OR 55-03-8P/BI

=> S 14 and ethanol  
 254437 ETHANOL  
 1124 ETHANOLS  
 254983 ETHANOL  
 (ETHANOL OR ETHANOLS)  
 L5 9 L4 AND ETHANOL

=> E "64-17-5"/BI,RN 25  
 E1 25 64-13-1P/BI  
 E2 5 64-15-3/BI  
 E3 197111 --> 64-17-5/BI  
 E4 0 64-17-5/RN  
 E5 1646 64-17-5D/BI  
 E6 530 64-17-5DP/BI

E7	15477	64-17-5P/BI
E8	34653	64-18-6/BI
E9	1342	64-18-6D/BI
E10	270	64-18-6DP/BI
E11	2172	64-18-6P/BI
E12	99042	64-19-7/BI
E13	5112	64-19-7D/BI
E14	884	64-19-7DP/BI
E15	7378	64-19-7P/BI
E16	1569	64-20-0/BI
E17	23	64-20-0D/BI
E18	7	64-20-0DP/BI
E19	17	64-20-0P/BI
E20	6	64-22-2/BI
E21	1	64-22-2P/BI
E22	5	64-24-4/BI
E23	19	64-26-6/BI
E24	8	64-27-7/BI
E25	1	64-30-6/BI

=> S E3  
 L6 197111 64-17-5/BI

=> s 16 and 14  
 L7 6 L6 AND L4

=> S L5 AND 1800<=PY<=1995  
 16758406 1800<=PY<=1995  
 L8 4 L5 AND 1800<=PY<=1995

=> DIS L8 1- IBIB IABS  
 YOU HAVE REQUESTED DATA FROM 4 ANSWERS - CONTINUE? Y/ (N) :Y  
 THE ESTIMATED COST FOR THIS REQUEST IS 10.96 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L8 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1995:833246 HCAPLUS  
 DOCUMENT NUMBER: 123:237845  
 TITLE: Liquid pharmaceutical compositions comprising thyroid hormones  
 INVENTOR(S): Dickinson, Jeffrey; Khan, Karrar Ahmad; Hague, John Neville; Smith, Alan  
 PATENT ASSIGNEE(S): Boots Co. PLC, UK  
 SOURCE: PCT Int. Appl., 21 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9520955	A1	19950810	WO 1995-EP323	19950130 <--
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US				
RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2182037	AA	19950810	CA 1995-2182037	19950130 <--
AU 9516631	A1	19950821	AU 1995-16631	19950130 <--
EP 742714	A1	19961120	EP 1995-908224	19950130
EP 742714	B1	20010328		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				

AT 200025	E	20010415	AT 1995-908224	19950130
ES 2155124	T3	20010501	ES 1995-908224	19950130
PT 742714	T	20010830	PT 1995-908224	19950130
ZA 9500743	A	19950801	ZA 1995-743	19950131 <--
US 6458842	B1	20021001	US 1996-682779	19960731
GR 3035706	T3	20010731	GR 2001-400554	20010405
US 2003130351	A1	20030710	US 2002-243555	20020913
US 6706255	B2	20040316	US 2004-802659	20040315
US 2004266877	A1	20041230	GB 1994-1891	A 19940201
PRIORITY APPLN. INFO.:				
			WO 1995-EP323	W 19950130
			US 1996-682779	A3 19960731
			US 2002-243555	A1 20020913

## ABSTRACT:

There is disclosed a liquid pharmaceutical composition comprising (1) one or more thyroid hormone, (2) 40-96 % ethanol by volume, (3) a pH-adjusting agent so that the measured pH of the composition is 9-12, and (4) 4-50 % water by volume, for the treatment of disorders associated with an impairment of the thyroid hormone functions. The liquid composition may be delivered by a metered dosage delivery system such as an aerosol or pump-action spray and provides improved patient compliance over traditional solid oral dosage forms. A solution contained Na levothyroxine 0.1, Na4EDTA 0.05, Na metabisulfite 0.05, Na saccharin 0.10%, \*\*\*ethanol\*\*\* 70, and purified water to 100% by volume

L8 ANSWER 2 OF 4 HCPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:467616 HCPLUS

DOCUMENT NUMBER: 101:67616

TITLE: Ethanol feeding and thyroid hormone monodeiodination

AUTHOR(S): Shank, M. L.; Singh, S. P.; Blivaiss, B. B.; Kabir, M. A.; Williams, K.; Premachandra, B. N.

CORPORATE SOURCE: Chicago Med. Sch., Univ. Health Sci., North Chicago, IL, 60064, USA

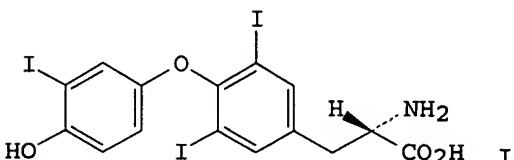
SOURCE: Metabolism, Clinical and Experimental (1984), 33(7), 667-71

CODEN: METAAJ; ISSN: 0026-0495

DOCUMENT TYPE: Journal

LANGUAGE: English

GRAPHIC IMAGE:



## ABSTRACT:

Adult male rats were placed on a 3-wk regime of EtOH [64-17-5] (as 20% of total calories) in a nutritionally adequate diet, and controls were matched equicalorically without EtOH. Serum measurements of T4 [55-03-8], T3 (I) [6893-02-3], FT4 [51-48-9], rT3 [5817-39-0], and TSH [9002-71-5] were performed in the fed and fasted state (18 h). In the fed state, serum hormone measurements did not differ between control and EtOH-treated rats. Overnight fasting had a significant effect in decreasing the serum I level in both exptl. and control rats and in decreasing the serum T4 level in EtOH-treated animals; FT4 and rT3 levels were not affected. Fasting also decreased in vitro hepatic T4 to I production to an equivalent degree in control and EtOH-treated rats, but did not alter hepatic T4 to rT3 production rates in control animals. In the fed state, hepatic rT3 neogenesis in animals given EtOH declined relative to the levels observed in control fed rats; fasting restored the

depressed rT3 neogenesis to the levels noted in the fed state. Because decreased rT3 production in EtOH-treated rats in the fed state could not be explained on the basis of a change in 5'-deiodinase activity, it is suggested that EtOH administered with a nutritionally adequate diet may inhibit hepatic rT3 generation by inhibiting T45-deiodinase.

L8 ANSWER 3 OF 4 HCPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1966:405179 HCPLUS  
 DOCUMENT NUMBER: 65:5179  
 ORIGINAL REFERENCE NO.: 65:988a-c  
 TITLE: Effect of thiouracil-type drugs on the  $\alpha$ -glycerophosphate dehydrogenase response to thyroxine analogs  
 AUTHOR(S): Hoffman, William W.; Richert, Dan A.; Westerfeld, W. W.  
 CORPORATE SOURCE: State Univ. of New York, Syracuse  
 SOURCE: Endocrinology (1966), 78(6), 1189-97  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ABSTRACT:  
 The response of mitochondrial  $\alpha$ -glycerophosphate dehydrogenase (GPD) activity to the injection of T4, T3, Tetrac, Triac, Tetraprop, Triprop, and isopropyl-T2 was determined in liver, kidney, and heart of weanling male rats maintained on a purified diet containing 2-thiouracil (TU). Similar studies were done with T4 and T3 in the presence of 6-propylthiouracil (PTU) and 2-mercapto-1-methylimidazole (MMI). TU inhibited the GPD response to T4 in all tissues, but did not decrease the response to T3 or the other analogs. PTU also inhibited T4 but not T3, while MMI had no effect on either. TU actually enhanced the GPD response to Tetraprop, Triprop, and isopropyl-T2, and in some cases the liver GPD response to Triac and T3. The effect of TU on the GPD responses to T4, T3, Tetrac, and Triac correlated well with the metabolic rate responses to these compounds. The extrathyroidal inhibition of T4 by thiouracils precludes the use of these drugs in antigoitrogenic assay procedures or in the estimation of endogenous T4 output. Such results with MMI appear to be valid for T4 and T3 since this drug also blocks synthesis in the gland but does not inhibit the peripheral effect of either compound. The peripheral inhibition of T4 by TU does not appear to be due to the incorporation of TU into the RNA of rat tissues, since the activities of all the analogs were not inhibited.

L8 ANSWER 4 OF 4 HCPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1966:29146 HCPLUS  
 DOCUMENT NUMBER: 64:29146  
 ORIGINAL REFERENCE NO.: 64:5437c-g  
 TITLE: Protozoan assays for vitamins, and cytotoxicity of carcinogens, and pharmacological agents  
 AUTHOR(S): Aaronson, A.; Baker, H.; Bensky, B.; Frank, O.; Zahalsky, A. C.  
 CORPORATE SOURCE: Roosevelt Hosp., New York, NY  
 SOURCE: Develop. Ind. Microbiol. (1965), Volume Date 1964, 6, 48-58  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ABSTRACT:  
 Protozoans were used for the assay of B vitamins in biol. samples of serum, urine, and tissues. The sensitivities of assays of thiamine, and biotin by using Ochromonas danica were, resp., 100 and 3 picograms/ml. The sensitivity limits of assays by using Tetrahymena pyriformis for nicotinic acid, vitamin B6, and pantothenic acid were 3 nanograms, 100 picograms, and 5 nanograms/ml., resp. O. malhamensis assayed vitamin B12 at a concentration of 1 picogram. T. pyriformis, and O. malhamensis were more specific for the several forms of nicotinic acid and vitamin B12. Of 19 different 1,2,4-triazoles tested against

O. danica, the most active compound was 3-amino-1,2,4-triazole, followed by 3-carboxy-5-amino-1,2,4-triazole, and 3-amino-carboxamino-5-phenyl-1,2,4-triazole, which were, resp., 2-, and 4-fold less inhibitory. Several metabolic sites of aminotriazole inhibition of O. danica were located. The carcinogen, 4-nitro-quinoline-N-oxide (I), 1 mg. %, completely inhibited the growth of O. danica, and Euglena gracilis, and the inhibition was annulled by L-tryptophan, apprx.4 mg. %, in both species. The tryptophan-transport system in protozoans was affected during I inhibition. The protozoan multiplication was inhibited to different degrees by hypocholesterolemic agents such as VOSO4, p-aminosalicylic acid,  $\alpha$ -phenylbutyric acid, Na L-thyroxinate, benzmalecene, triparanol (MER-29), 22,25-diazocholestanol,  $\beta$ -diethylaminoethyldiphenylpropylacetate (SKF-525A), 2,2 diphenyl-1- $\beta$ -dimethylaminoethoxypentane (SKF-3301A), trans-3-[p-diethylaminoethoxy]phenyl]-2-phenyl-2-pentenenitrile (P-3013), and trans-3-(p-chlorophenyl)-2-(p-diethylaminoethoxy)-phenyl-2-pentenenitrile (P-3429). Oleic acid overcame inhibition of O. danica by a variety of above-named compds. with different inhibitory sites on mammalian sterol biosynthesis. The major sites of action of several hypocholesterolemic agents on sterol-synthesizing microorganisms, *Saccharomyces cerevisiae*, *E. gracilis*, and *O. danica*, and in nonsterol-synthesizing microorganisms, *T. pyriformis*, *Rhodopseudomonas palustris*, and *Coccochloris elabens*, was apparently on the metabolism of unsatd. fatty acids rather than sterol metabolism. Unsatd. but not saturated fatty acids annulled the inhibition of *Ochromonas* respiration induced by several hypocholesterolemic agents.

=> E DICKINSON J/AU 25

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E2	1	DICKINSON INGRAM/AU
E3	10	--> DICKINSON J/AU
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E5	2	DICKINSON JEFFREY ALAN/AU
E6	4	DICKINSON JEFFREY W/AU
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E8	1	DICKINSON JENNIFER/AU
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E11	1	DICKINSON JENNY A/AU
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E20	5	DICKINSON JOHN/AU
E21	9	DICKINSON JOHN A/AU
E22	2	DICKINSON JOHN C/AU
E23	4	DICKINSON JOHN D/AU
E24	11	DICKINSON JOHN G/AU
E25	6	DICKINSON JOHN O/AU

=> S (E3) AND (THYROID OR THYRONINE OR LEVOTHYROXINE OR TETRAIODOTHYRONINE)

3 "DICKINSON JEFFREY"/AU

79467 THYROID

2955 THYROIDS

79814 THYROID

(THYROID OR THYROIDS)

2184 THYRONINE

239 THYRONINES

2318 THYRONINE

(THYRONINE OR THYRONINES)

503 LEVOTHYROXINE

235 TETRAIODOTHYRONINE

7 TETRAIODOTHYRONINES

242 TETRAIODOTHYRONINE

(TETRAIODOTHYRONINE OR TETRAIODOTHYRONINES)

L9 1 ("DICKINSON JEFFREY"/AU) AND (THYROID OR THYRONINE OR LEVOTHYROXINE OR TETRAIODOTHYRONINE)

=> DIS L9 1 TI

L9 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN

TI Liquid pharmaceutical compositions comprising thyroid hormones

=> DIS L9 1 IBIB

THE ESTIMATED COST FOR THIS REQUEST IS 1.14 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L9 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:833246 HCAPLUS

DOCUMENT NUMBER: 123:237845

TITLE: Liquid pharmaceutical compositions comprising thyroid hormones

INVENTOR(S): Dickinson, Jeffrey; Khan, Karrar Ahmad; Hague, John Neville; Smith, Alan

PATENT ASSIGNEE(S): Boots Co. PLC, UK

SOURCE: PCT Int. Appl., 21 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9520955	A1	19950810	WO 1995-EP323	19950130
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT,				

UA, US  
 RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU,  
 MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN,  
 TD, TG

CA 2182037	AA	19950810	CA 1995-2182037	19950130
AU 9516631	A1	19950821	AU 1995-16631	19950130
EP 742714	A1	19961120	EP 1995-908224	19950130
EP 742714	B1	20010328		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
AT 200025	E	20010415	AT 1995-908224	19950130
ES 2155124	T3	20010501	ES 1995-908224	19950130
PT 742714	T	20010830	PT 1995-908224	19950130
ZA 9500743	A	19950801	ZA 1995-743	19950131
US 6458842	B1	20021001	US 1996-682779	19960731
GR 3035706	T3	20010731	GR 2001-400554	20010405
US 2003130351	A1	20030710	US 2002-243555	20020913
US 6706255	B2	20040316		
US 2004266877	A1	20041230	US 2004-802659	20040315
PRIORITY APPLN. INFO.:				
			GB 1994-1891	A 19940201
			WO 1995-EP323	W 19950130
			US 1996-682779	A3 19960731
			US 2002-243555	A1 20020913

=> E KHAN KARRAR/AU 25

E1	2	KHAN KARIM M/AU
E2	6	KHAN KARL/AU
E3	1	--> KHAN KARRAR/AU
E4	15	KHAN KARRAR A/AU
E5	5	KHAN KARRAR AHMAD/AU
E6	3	KHAN KARRAR AHMED/AU
E7	1	KHAN KASHIF/AU
E8	1	KHAN KASHIF A/AU
E9	2	KHAN KASHIF AZIZ/AU
E10	2	KHAN KH/AU
E11	1	KHAN KHA SOK/AU
E12	1	KHAN KHAIRUL ALAM/AU
E13	14	KHAN KHALEQUE NEWAZ/AU
E14	16	KHAN KHALID/AU
E15	11	KHAN KHALID A/AU
E16	1	KHAN KHALID AZIZ/AU
E17	3	KHAN KHALID H/AU
E18	3	KHAN KHALID HAFIZ/AU
E19	70	KHAN KHALID M/AU
E20	3	KHAN KHALID MAHMOOD/AU
E21	3	KHAN KHALID MOHAMMAD/AU
E22	53	KHAN KHALID MOHAMMED/AU
E23	7	KHAN KHALID S/AU
E24	2	KHAN KHALID SAEED/AU
E25	2	KHAN KHALID SAIFULLAH/AU

=> S (E3 OR E4 OR E5 OR E6) AND (THYROID OR THYRONINE OR LEVOTHYROXINE OR TETRAIODOTHYRONINE)

1	"KHAN KARRAR"/AU
15	"KHAN KARRAR A"/AU
5	"KHAN KARRAR AHMAD"/AU
3	"KHAN KARRAR AHMED"/AU

79467 THYROID

2955 THYROIDS

79814 THYROID

(THYROID OR THYROIDS)

2184 THYRONINE

239 THYRONINES

2318 THYRONINE

(THYRONINE OR THYRONINES)

503 LEVOTHYROXINE

235 TETRAIODOTHYRONINE  
7 TETRAIODOTHYRONINES  
242 TETRAIODOTHYRONINE

(TETRAIODOTHYRONINE OR TETRAIODOTHYRONINES)

L10 3 ("KHAN KARRAR"/AU OR "KHAN KARRAR A"/AU OR "KHAN KARRAR AHMAD"/AU OR "KHAN KARRAR AHMED"/AU) AND (THYROID OR THYRONINE OR LEVOTHYROXINE OR TETRAIODOTHYRONINE)

=> DIS L10 1 IBIB IABS

THE ESTIMATED COST FOR THIS REQUEST IS 2.74 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L10 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:856178 HCAPLUS

DOCUMENT NUMBER: 123:237848

TITLE: Pharmaceutical compositions containing thyroid hormones

INVENTOR(S): Khan, Karrar Ahmad; Smith, Alan

PATENT ASSIGNEE(S): Boots Co. PLC, UK

SOURCE: PCT Int. Appl., 19 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9520953	A1	19950810	WO 1995-EP321	19950130
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US				
RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2182038	AA	19950810	CA 1995-2182038	19950130
AU 9515370	A1	19950821	AU 1995-15370	19950130
EP 732920	A1	19960925	EP 1995-907000	19950130
EP 732920	B1	20031029		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
AT 252899	E	20031115	AT 1995-907000	19950130
ES 2210282	T3	20040701	ES 1995-907000	19950130
ZA 9500741	A	19950801	ZA 1995-741	19950131
US 5753254	A	19980519	US 1996-682783	19960731
PRIORITY APPLN. INFO.:			GB 1994-1892	A 19940201
			WO 1995-EP321	W 19950130

ABSTRACT:

A solid fast dispersing dosage form of a pharmaceutical composition suitable for oral administration comprises one or more compound thyroid hormone or hormones; from about 80% to about 99.9% of disintegrating agent; from about 0.01% to about 10% of flavoring agent; and from about 0.1% to about 5% of lubricating agent; which is used in the treatment of disorders associated with the improvement of the thyroid hormone function. A fast dispersing tablet contained levothyroxine 50 $\mu$ g, maize starch powder 67.30, microcryst. cellulose 30.00, citric acid powder 2.00, aspartame 0.200, and Mg stearate 0.500%.

=> DIS L10 2 IBIB IABS

L10 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:856177 HCAPLUS

DOCUMENT NUMBER: 123:237847

TITLE: Pharmaceutical chewable tablets containing

INVENTOR(S): thyroid hormones  
 Khan, Karrar Ahmad; Smith, Alan  
 PATENT ASSIGNEE(S): Boots Co. PLC, UK  
 SOURCE: PCT Int. Appl., 19 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9520954	A1	19950810	WO 1995-EP322	19950130
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US				
RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9516630	A1	19950821	AU 1995-16630	19950130
ZA 9500472	A	19950801	ZA 1995-472	19950131
PRIORITY APPLN. INFO.:			GB 1994-1879	A 19940201
			WO 1995-EP322	W 19950130

## ABSTRACT:

Suckable, swallowable and chewable oral dosage forms of a pharmaceutical composition suitable for oral administration comprises at least one thyroid hormone; from about 60 % to about 90 % of an inert diluent which is a sugar or sugar alc.; from about 5 % to about 35 % of disintegrating agent; and from about 0.1 % to about 5 % of a lubricating agent for the treatment of disorders associated with the improvement of the thyroid hormone function. A chewable tablet contained levothyroxine 50 $\mu$ g, maize starch 12, microcryst. cellulose 10, citric acid 1.5, sucrose 76, and Mg stearate 0.5%.

=> DIS L10 3 IBIB IABS

L10 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1995:833246 HCAPLUS  
 DOCUMENT NUMBER: 123:237845  
 TITLE: Liquid pharmaceutical compositions comprising thyroid hormones  
 INVENTOR(S): Dickinson, Jeffrey; Khan, Karrar Ahmad;  
 Hague, John Neville; Smith, Alan  
 PATENT ASSIGNEE(S): Boots Co. PLC, UK  
 SOURCE: PCT Int. Appl., 21 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9520955	A1	19950810	WO 1995-EP323	19950130
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US				
RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2182037	AA	19950810	CA 1995-2182037	19950130
AU 9516631	A1	19950821	AU 1995-16631	19950130

EP 742714	A1	19961120	EP 1995-908224	19950130
EP 742714	B1	20010328		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
AT 200025	E	20010415	AT 1995-908224	19950130
ES 2155124	T3	20010501	ES 1995-908224	19950130
PT 742714	T	20010830	PT 1995-908224	19950130
ZA 9500743	A	19950801	ZA 1995-743	19950131
US 6458842	B1	20021001	US 1996-682779	19960731
GR 3035706	T3	20010731	GR 2001-400554	20010405
US 2003130351	A1	20030710	US 2002-243555	20020913
US 6706255	B2	20040316		
US 2004266877	A1	20041230	US 2004-802659	20040315
PRIORITY APPLN. INFO.:			GB 1994-1891	A 19940201
			WO 1995-EP323	W 19950130
			US 1996-682779	A3 19960731
			US 2002-243555	A1 20020913

## ABSTRACT:

There is disclosed a liquid pharmaceutical composition comprising (1) one or more \*\*\*thyroid\*\*\* hormone, (2) 40-96 % ethanol by volume, (3) a pH-adjusting agent so that the measured pH of the composition is 9-12, and (4) 4-50 % water by volume, for the treatment of disorders associated with an impairment of the \*\*\*thyroid\*\*\* hormone functions. The liquid composition may be delivered by a metered dosage delivery system such as an aerosol or pump-action spray and provides improved patient compliance over traditional solid oral dosage forms. A solution contained Na levothyroxine 0.1, Na4EDTA 0.05, Na metabisulfite 0.05, Na saccharin 0.10%, ethanol 70, and purified water to 100% by volume

=> E HAGUE JOHN/AU 25

E1	1	HAGUE JAYNE A/AU
E2	1	HAGUE JOE/AU
E3	0 -->	HAGUE JOHN/AU
E4	1	HAGUE JOHN F/AU
E5	14	HAGUE JOHN L/AU
E6	2	HAGUE JOHN M/AU
E7	1	HAGUE JOHN N/AU
E8	2	HAGUE JOHN NEVILLE/AU
E9	1	HAGUE JONATHAN D/AU
E10	9	HAGUE JONATHAN DAVID/AU
E11	1	HAGUE JONATHAN DAVIDE/AU
E12	1	HAGUE JONATHAN F E/AU
E13	1	HAGUE JONATHON DAVID/AU
E14	1	HAGUE KATHLEEN/AU
E15	1	HAGUE KATHLEEN L/AU
E16	1	HAGUE KAZI E/AU
E17	2	HAGUE KEITH/AU
E18	1	HAGUE KIMBERLY A/AU
E19	1	HAGUE L K/AU
E20	1	HAGUE LISA/AU
E21	2	HAGUE LISA K/AU
E22	1	HAGUE LISA M/AU
E23	15	HAGUE LOUISE D/AU
E24	1	HAGUE LOUISE DENTLER/AU
E25	2	HAGUE LYNDA/AU

=> S (E4 OR E7 OR E8) AND (THYROID OR THYRONINE OR LEVOTHYROXINE OR TETRAIODOHYRONINE)

1 "HAGUE JOHN F"/AU
1 "HAGUE JOHN N"/AU
2 "HAGUE JOHN NEVILLE"/AU

79467 THYROID

2955 THYROIDS

79814 THYROID

(THYROID OR THYROIDS)

2184 THYRONINE  
 239 THYRONINES  
 2318 THYRONINE  
 (THYRONINE OR THYRONINES)  
 503 LEVOTHYROXINE  
 235 TETRAIODOTHYRONINE  
 7 TETRAIODOTHYRONINES  
 242 TETRAIODOTHYRONINE  
 (TETRAIODOTHYRONINE OR TETRAIODOTHYRONINES)  
 L11 1 ("HAGUE JOHN F"/AU OR "HAGUE JOHN N"/AU OR "HAGUE JOHN NEVILLE"/AU) AND  
 (THYROID OR THYRONINE OR LEVOTHYROXINE OR TETRAIODOTHYRONINE)

=> DIS L11 1 SAM

L11 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN  
 IC ICM A61K031-195  
 ICS A61K009-00; A61K047-10  
 CC 63-6 (Pharmaceuticals)  
 TI Liquid pharmaceutical compositions comprising thyroid hormones  
 ST thyroid hormone oral soln  
 IT Thyroid hormones  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (liquid pharmaceuticals containing thyroid hormones)  
 IT Pharmaceutical dosage forms  
 (liqs., liquid pharmaceuticals containing thyroid hormones)  
 IT 51-48-9, Levothyroxine, biological studies 55-03-8,  
 Levothyroxine sodium 64-17-5, Ethanol, biological studies  
 1041-01-6, L-3,5-Diiodothyronine 5817-39-0 6893-02-3, Liothyronine  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (liquid pharmaceuticals containing thyroid hormones)

=> E SMITH ALAN/AU 25

E1 6 SMITH AL/AU  
 E2 4 SMITH AL J JR/AU  
 E3 138 --> SMITH ALAN/AU  
 E4 9 SMITH ALAN A/AU  
 E5 7 SMITH ALAN ARTHUR/AU  
 E6 45 SMITH ALAN B/AU  
 E7 1 SMITH ALAN BRADFORD/AU  
 E8 4 SMITH ALAN C/AU  
 E9 8 SMITH ALAN C B/AU  
 E10 3 SMITH ALAN CAMERON/AU  
 E11 4 SMITH ALAN CHARLES BRANDON/AU  
 E12 1 SMITH ALAN CHRISTOPHER/AU  
 E13 8 SMITH ALAN CRAIG/AU  
 E14 15 SMITH ALAN D/AU  
 E15 141 SMITH ALAN E/AU  
 E16 2 SMITH ALAN E W/AU  
 E17 1 SMITH ALAN EARL/AU  
 E18 7 SMITH ALAN EDWARD/AU  
 E19 1 SMITH ALAN ERNEST W/AU  
 E20 8 SMITH ALAN F/AU  
 E21 34 SMITH ALAN G/AU  
 E22 3 SMITH ALAN GILBERT/AU  
 E23 2 SMITH ALAN GUY/AU  
 E24 1 SMITH ALAN H/AU  
 E25 2 SMITH ALAN HANSON/AU

=> S (E3) AND (THYROID OR THYRONINE OR LEVOTHYROXINE OR TETRAIODOTHYRONINE)  
 138 "SMITH ALAN"/AU  
 79467 THYROID  
 2955 THYROIDS  
 79814 THYROID  
 (THYROID OR THYROIDS)

2184 THYRONINE  
 239 THYRONINES  
 2318 THYRONINE  
 (THYRONINE OR THYRONINES)  
 503 LEVOTHYROXINE  
 235 TETRAIODOTHYRONINE  
 7 TETRAIODOTHYRONINES  
 242 TETRAIODOTHYRONINE  
 (TETRAIODOTHYRONINE OR TETRAIODOTHYRONINES)  
 L12 3 ("SMITH ALAN"/AU) AND (THYROID OR THYRONINE OR LEVOTHYROXINE OR TETRAIODOTHYRONINE)

=> DIS L12 1- SAM

YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):Y

L12 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN  
 IC ICM A61K031-195  
 ICS A61K009-00  
 CC 63-6 (Pharmaceuticals)  
 TI Pharmaceutical compositions containing thyroid hormones  
 ST pharmaceutical compn thyroid hormone; levothyroxine  
 pharmaceutical tablet  
 IT Flavoring materials  
 (pharmaceutical compns. containing thyroid hormones)  
 IT Bentonite, biological studies  
 Thyroid hormones  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (pharmaceutical compns. containing thyroid hormones)  
 IT Pharmaceutical dosage forms  
 (solids, oral, pharmaceutical compns. containing thyroid  
 hormones)  
 IT Pharmaceutical dosage forms  
 (tablets, pharmaceutical compns. containing thyroid hormones)  
 IT 51-48-9, biological studies 55-03-8, Levothyroxine sodium  
 151-21-3, Sodium lauryl sulfate, biological studies 1041-01-6,  
 L-3,5-Diiodothyronine 5817-39-0 6893-02-3 9000-30-0, Guar gum  
 9002-18-0, Agar 9004-32-4, Carboxymethyl cellulose 9004-34-6,  
 Cellulose, biological studies 9004-67-5, Methyl Cellulose 9005-25-8,  
 Starch, biological studies 9005-32-7, Alginic acid  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (pharmaceutical compns. containing thyroid hormones)

L12 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN  
 IC ICM A61K031-195  
 ICS A61K009-00  
 CC 63-6 (Pharmaceuticals)  
 TI Pharmaceutical chewable tablets containing thyroid hormones  
 ST pharmaceutical chewable tablet thyroid hormone;  
 levothyroxine pharmaceutical chewable tablet  
 IT Flavoring materials  
 (pharmaceutical chewable tablets containing thyroid hormones)  
 IT Bentonite, biological studies  
 Thyroid hormones  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (pharmaceutical chewable tablets containing thyroid hormones)  
 IT Pharmaceutical dosage forms  
 (solids, oral, pharmaceutical chewable tablets containing thyroid  
 hormones)  
 IT Pharmaceutical dosage forms  
 (tablets, chewable, pharmaceutical chewable tablets containing  
 thyroid hormones)  
 IT 51-48-9, biological studies 55-03-8, Levothyroxine sodium  
 151-21-3, Sodium lauryl sulfate, biological studies 1041-01-6,  
 L-3,5-Diiodothyronine 5817-39-0 6893-02-3 9000-30-0, Guar gum  
 9002-18-0, Agar 9004-32-4, Carboxymethyl cellulose 9004-34-6,

Cellulose, biological studies 9004-67-5, Methyl Cellulose 9005-25-8,  
 Starch, biological studies 9005-32-7, Alginic acid  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (pharmaceutical chewable tablets containing thyroid hormones)

L12 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN  
 IC ICM A61K031-195  
 ICS A61K009-00; A61K047-10  
 CC 63-6 (Pharmaceuticals)  
 TI Liquid pharmaceutical compositions comprising thyroid hormones  
 ST thyroid hormone oral soln  
 IT Thyroid hormones  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (liquid pharmaceuticals containing thyroid hormones)  
 IT Pharmaceutical dosage forms  
 (liqs., liquid pharmaceuticals containing thyroid hormones)  
 IT 51-48-9, Levothyroxine, biological studies 55-03-8,  
 Levothyroxine sodium 64-17-5, Ethanol, biological studies  
 1041-01-6, L-3,5-Diiodothyronine 5817-39-0 6893-02-3, Liothyronine  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (liquid pharmaceuticals containing thyroid hormones)

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	72.57	162.02
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-5.25	-5.25

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	3.57	165.59
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-5.25

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L13 1 5817-39-0/RN

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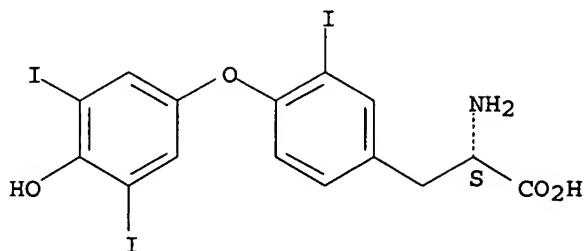
NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

=> D L13 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y  
THE ESTIMATED COST FOR THIS REQUEST IS 6.36 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/(N):y

L13 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 5817-39-0 REGISTRY  
CN L-Tyrosine, O-(4-hydroxy-3,5-diodophenyl)-3-iodo- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Alanine, 3-[4-(4-hydroxy-3,5-diodophenoxy)-3-iodophenyl]-, L- (8CI)  
OTHER NAMES:  
CN 3',5',3-Triiodothyronine  
CN 3,3',5'-L-Triiodothyronine  
CN 3,3',5'-T3  
CN 3,3',5'-Triodo-L-thyronine  
CN 3,3',5'-Triiodothyronine  
CN Isoliotyronine  
CN Reverse L-triiodothyronine  
CN Reverse T3  
CN Reverse triiodothyronine  
CN rT3  
FS STEREOSEARCH  
DR 2820-50-0  
MF C15 H12 I3 N 04  
CI COM  
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN\*, BIOSIS, BIOTECHNO,  
CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CSCHEM, DDFU, DRUGU, EMBASE, IPA,  
MEDLINE, PROMT, TOXCENTER, USPAT2, USPATFULL  
(\*File contains numerically searchable property data)  
DT.CA CPlus document type: Conference; Dissertation; Journal; Patent; Report  
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);  
PREP (Preparation); USES (Uses)  
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological  
study); PREP (Preparation); USES (Uses)  
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological  
study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP  
(Preparation); PROC (Process); PRP (Properties); RACT (Reactant or  
reagent); USES (Uses); NORL (No role in record)  
RLD.NP Roles for non-specific derivatives from non-patents: BIOL (Biological  
study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP  
(Preparation); PRP (Properties)

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1607 REFERENCES IN FILE CA (1907 TO DATE)  
 4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 1608 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND  
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=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.78	168.37
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-5.25

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STRUCTURE FILE UPDATES: 4 SEP 2006 HIGHEST RN 905816-92-4  
 DICTIONARY FILE UPDATES: 4 SEP 2006 HIGHEST RN 905816-92-4

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<http://www.cas.org/ONLINE/UG/regprops.html>

=> S 6893-02-3/RN

L14

1 6893-02-3/RN

=> SET NOTICE 1 DISPLAY

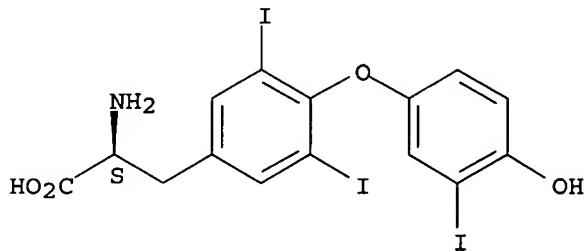
NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND  
SET COMMAND COMPLETED

=> D L14 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y  
THE ESTIMATED COST FOR THIS REQUEST IS 6.36 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L14 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 6893-02-3 REGISTRY  
CN L-Tyrosine, O-(4-hydroxy-3-iodophenyl)-3,5-diiodo- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Alanine, 3-[4-(4-hydroxy-3-iodophenoxy)-3,5-diiodophenyl]-, L- (8CI)  
CN Thyronine, 3,3',5-triiodo-, L- (6CI)  
OTHER NAMES:  
CN 3,3',5-Triiodo-L-thyronine  
CN 3,3',5-Triiodothyronine  
CN 3,5,3'-Triiodothyronine  
CN 4-(4-Hydroxy-3-iodophenoxy)-3,5-diiodophenylalanine  
CN Cyronine  
CN L-3,3',5-Triiodothyronine  
CN L-Liothyronine  
CN L-T3  
CN L-Triiodothyronine  
CN Liothyronin  
CN Liothyronine  
CN NSC 80203  
CN T3  
CN T3 (amino acid)  
CN T3 (Hormone)  
CN Tresitope  
CN Triiodo-L-thyronine  
CN Triiodothyronine  
FS STEREOSEARCH  
DR 7013-53-8, 57164-27-9  
MF C15 H12 I3 N 04  
CI COM  
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN\*, BIOSIS,  
BIOTECHNO, CA, CABAB, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMLIST,  
CIN, CSCHEM, CSNB, DDFU, DRUGU, EMBASE, GMELIN\*, HSDB\*, IFICDB, IFIPAT,  
IFIUDB, IPA, MEDLINE, MRCK\*, NAPRALERT, PROMT, PS, RTECS\*, SCISEARCH,  
SPECINFO, TOXCENTER, USAN, USPAT2, USPATFULL, VETU  
(\*File contains numerically searchable property data)  
Other Sources: EINECS\*\*, WHO  
(\*\*Enter CHEMLIST File for up-to-date regulatory information)  
DT.CA CAplus document type: Book; Conference; Dissertation; Journal; Patent;  
Report  
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);  
OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties);  
RACT (Reactant or reagent); USES (Uses); NORL (No role in record)  
RLD.P Roles for non-specific derivatives from patents: ANST (Analytical  
study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP  
(Properties); RACT (Reactant or reagent); USES (Uses)  
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological  
study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU  
(Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT  
(Reactant or reagent); USES (Uses); NORL (No role in record)  
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical  
study); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU  
(Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT  
(Reactant or reagent); USES (Uses)

Absolute stereochemistry. Rotation (+).



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

18892 REFERENCES IN FILE CA (1907 TO DATE)  
 159 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 18907 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
 21 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND  
 SET COMMAND COMPLETED

=>

=> FIL HOME			
COST IN U.S. DOLLARS	SINCE FILE	TOTAL	
FULL ESTIMATED COST	ENTRY	SESSION	
	2.78	171.15	
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL	
CA SUBSCRIBER PRICE	ENTRY	SESSION	
	0.00	-5.25	

FILE 'HOME' ENTERED AT 10:02:48 ON 05 SEP 2006

=> d his

(FILE 'HOME' ENTERED AT 09:15:43 ON 05 SEP 2006)

FILE 'BIOSIS' ENTERED AT 09:15:53 ON 05 SEP 2006

FILE 'REGISTRY' ENTERED AT 09:16:13 ON 05 SEP 2006

L1	E "LEVOTHYROXINE"/CN 25
	2 S E3 OR E4
	E "LEVOTHYROXINE"/CN 25
	E "LIOTHRONINE"/CN 25
	E "TRIIODOTHYRONINE"/CN 25
L2	9 S E3 OR E12 OR E13 OR E14 OR E15 OR E16 OR E19 OR E20 OR E21 OR
	E "DIIODOTHYRONINE"/CN 25
L3	1 S E3

FILE 'HOME' ENTERED AT 09:23:41 ON 05 SEP 2006

FILE 'HCAPLUS' ENTERED AT 09:38:19 ON 05 SEP 2006

L4	E "55-03-8"/BI,RN 25
	481 S E3 OR E5
L5	9 S L4 AND ETHANOL
	E "64-17-5"/BI,RN 25
L6	197111 S E3

L7           6 S L6 AND L4  
 L8           4 S L5 AND 1800<=PY<=1995  
             E DICKINSON J/AU 25  
             E DICKINSON JEFFREY/AU 25  
 L9           1 S (E3) AND (THYROID OR THYRONINE OR LEVOTHYROXINE OR TETRAIODOT  
             E KHAN KARRAR/AU 25  
 L10          3 S (E3 OR E4 OR E5 OR E6) AND (THYROID OR THYRONINE OR LEVOTHYRO  
             E HAGUE JOHN/AU 25  
 L11          1 S (E4 OR E7 OR E8) AND (THYROID OR THYRONINE OR LEVOTHYROXINE O  
             E SMITH ALAN/AU 25  
 L12          3 S (E3) AND (THYROID OR THYRONINE OR LEVOTHYROXINE OR TETRAIODOT

FILE 'HOME' ENTERED AT 09:50:33 ON 05 SEP 2006

FILE 'REGISTRY' ENTERED AT 10:00:41 ON 05 SEP 2006

L13          1 S 5817-39-0/RN  
             SET NOTICE 1 DISPLAY  
             SET NOTICE LOGIN DISPLAY

FILE 'REGISTRY' ENTERED AT 10:01:52 ON 05 SEP 2006

L14          1 S 6893-02-3/RN  
             SET NOTICE 1 DISPLAY  
             SET NOTICE LOGIN DISPLAY

FILE 'HOME' ENTERED AT 10:02:48 ON 05 SEP 2006

=>  
 =>  
 =>  
 =>

=> s (Berlthyrox or Dathroid or Droxine or Eferox or thyroxine or Laevoxin or Letrox or Levoroxine or Levotirox or Levotiroxina or Levoxyl or Synthroid or Thyradin or Thyrex or Thevier or Throxinique or Thyradin or Thyrax) and ethanol  
 THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

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=> FIL HCAPLUS			
COST IN U.S. DOLLARS	SINCE FILE	TOTAL	
	ENTRY	SESSION	
FULL ESTIMATED COST	26.46	197.61	
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL	
	ENTRY	SESSION	
CA SUBSCRIBER PRICE	0.00	-5.25	

FILE 'HCAPLUS' ENTERED AT 11:18:21 ON 05 SEP 2006  
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FILE COVERS 1907 - 5 Sep 2006 VOL 145 ISS 11

FILE LAST UPDATED: 4 Sep 2006 (20060904/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s (Berlthyrox or Dathroid or Droxine or Eferox or thyroxine or Laevoxin or Letrox or Levoroxine or Levotirox or Levotiroxina or Levoxyl or Synthroid or Thyradin or Thyrex or Thevier or Throxinique or Thyradin or Thyrax) and ethanol

0 BERLTHYROX  
 0 DATHROID  
 0 DROXINE  
 1 EFEROX  
 30827 THYROXINE  
 56 THYROXINES  
 30835 THYROXINE  
 (THYROXINE OR THYROXINES)  
 0 LAEVOXIN  
 0 LETROX  
 0 LEVOROXINE  
 0 LEVOTIROX  
 0 LEVOTIROXINA  
 5 LEVOXYL  
 26 SYNTHROID  
 32 THYRADIN  
 4 THYREX  
 0 THEVIER  
 0 THROXINIQUE  
 32 THYRADIN  
 3 THYRAX  
 254437 ETHANOL  
 1124 ETHANOLS  
 254983 ETHANOL

(ETHANOL OR ETHANOLS)

L15 188 (BERLTHYROX OR DATHROID OR DROXINE OR EFEROX OR THYROXINE OR LAEVOXIN OR LETROX OR LEVOROXINE OR LEVOTIROX OR LEVOTIROXINA OR LEVOXYL OR SYNTHROID OR THYRADIN OR THYREX OR THEVIER OR THROX INIQUE OR THYRADIN OR THYRAX) AND ETHANOL

=> S L15 AND 1800<=PY<=1995

16758406 1800&lt;=PY&lt;=1995

L16 133 L15 AND 1800<=PY<=1995

=> S L16 AND (PHARMAC?)

570298 PHARMAC?

L17 9 L16 AND (PHARMAC?)

=> DIS L17 1 SAM IBIB IABS

THE ESTIMATED COST FOR THIS REQUEST IS 3.07 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L17 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

CC 1-3 (Pharmacology)

TI Non-congeneric structure-pharmacokinetic property correlation studies using fuzzy adaptive least-squares: oral bioavailability

ST structure pharmacokinetic correlation bioavailability simulation

IT Quantitative structure-activity relationship  
 (in drug oral bioavailability simulation)IT Simulation and Modeling, biological  
 (of drug oral bioavailability, non-congeneric structure-pharmacokinetic property correlation in)IT Pharmacokinetics  
 (of drugs, structure and oral bioavailability in relation to)

IT Drug bioavailability

(simulation of oral, non-congeneric structure-pharmacokinetic property correlation in)

IT Molecular structure-biological activity relationship  
 (pharmacokinetic, in drug oral bioavailability simulation)

IT 50-02-2, Dexamethasone 50-06-6, Phenobarbital, biological studies  
 50-18-0, Cyclophosphamide 50-24-8, Prednisolone 50-33-9,  
 Phenylbutazone, biological studies 50-36-2, Cocaine 50-44-2,  
 Mercaptopurine 50-47-5, Desipramine 50-48-6, Amitriptyline 50-49-7,  
 Imipramine 50-53-3, biological studies 50-78-2, Acetylsalicylic acid  
 51-06-9, Procainamide 51-21-8, Fluorouracil 51-34-3, Scopolamine  
 51-48-9, L-Thyroxine, biological studies 51-55-8, Atropine,  
 biological studies 52-01-7, Spironolactone 52-53-9, Verapamil  
 52-86-8, Haloperidol 53-03-2 53-86-1, Indomethacin 54-05-7,  
 Chloroquine 54-11-5, Nicotine 54-31-9, Furosemide 55-63-0,  
 Nitroglycerin 56-29-1, Hexobarbital 56-54-2, Quinidine 56-75-7,  
 Chloramphenicol 57-27-2, Morphine, biological studies 57-41-0,  
 Phenytoin 57-42-1, Meperidine 57-66-9, Probenecid 57-96-5,  
 Sulfinpyrazone 58-08-2, Caffeine, biological studies 58-25-3,  
 Chlordiazepoxide 58-55-9, Theophylline, biological studies 58-73-1  
 58-93-5, Hydrochlorothiazide 59-05-2, Methotrexate 59-41-6, Bretylium  
 60-54-8, Tetracycline 61-33-6, Benzylpenicillin, biological studies  
 61-72-3, Cloxacillin 64-17-5, Ethanol, biological studies  
 64-77-7, Tolbutamide 66-79-5, Oxacillin 68-35-9, Sulfadiazine  
 69-53-4, Ampicillin 69-72-7, Salicylic acid, biological studies  
 71-63-6, Digitoxin 72-69-5, Nortriptyline 74-55-5, Ethambutol  
 76-57-3, Codeine 76-99-3, Methadone 77-36-1, Chlorthalidone 77-67-8,  
 Ethosuximide 80-08-0 81-81-2, Warfarin 83-43-2, Methylprednisolone  
 86-54-4, Hydralazine 87-08-1, Phenoxymethylenicillin 87-33-2,  
 Isosorbide dinitrate 90-89-1, Diethylcarbamazine 94-20-2,  
 Chlorpropamide 99-66-1, Valproic acid 100-33-4, Pentamidine  
 103-90-2, Acetaminophen 113-92-8 114-07-8, Erythromycin 125-33-7,  
 Primidone 127-69-5, Sulfoxazole 129-20-4, Oxyphenbutazone  
 130-95-0, Quinine 137-58-6, Lidocaine 146-22-5 147-52-4, Nafcillin  
 147-94-4, Cytarabine 148-82-3, Melphalan 155-97-5, Pyridostigmine  
 298-46-4, Carbamazepine 298-50-0, Propantheline 305-03-3, Chlorambucil  
 315-30-0, Allopurinol 359-83-1, Pentazocine 364-62-5, Metoclopramide  
 364-98-7, Diazoxide 378-44-9, Betamethasone 396-01-0, Triamterene  
 438-60-8, Protriptyline 439-14-5, Diazepam 443-48-1, Metronidazole  
 446-86-6, Azathioprine 465-65-6, Naloxone 525-66-6, Propranolol  
 555-30-6, Methyldopa 564-25-0, Doxycycline 604-75-1 637-07-0,  
 Clofibrate 657-24-9, Metformin 738-70-5, Trimethoprim 768-94-5,  
 Amantadine 846-49-1, Lorazepam 846-50-4, Temazepam 1088-11-5,  
 Desmethyldiazepam 1622-61-3, Clonazepam 1622-62-4, Flunitrazepam  
 1668-19-5, Doxepin 1951-25-3, Amiodarone 1972-08-3,  
 Tetrahydrocannabinol 2022-85-7, Flucytosine 2062-78-4, Pimozide  
 3116-76-5, Dicloxacillin 3737-09-5, Disopyramide 4205-90-7, Clonidine  
 5250-39-5, Flucloxacillin 6452-71-7, Oxprenolol 6493-05-6,  
 Pentoxyfylline 6740-88-1, Ketamine 6893-02-3, Triiodothyronine  
 7206-76-0, Phenylethylmalonamide 10118-90-8, Minocycline 10262-69-8,  
 Maprotiline 13523-86-9, Pindolol 13655-52-2, Alprenolol 15307-86-5,  
 Diclofenac 15686-71-2, Cephalexin 15687-27-1, Ibuprofen 16051-77-7,  
 Isosorbide-5-mononitrate 16106-20-0, Isosorbide-2-mononitrate  
 16590-41-3, Naltrexone 18323-44-9, Clindamycin 19216-56-9, Prazosin  
 19794-93-5, Trazodone 20594-83-6, Nalbuphine 20830-75-5, Digoxin  
 21829-25-4, Nifedipine 22071-15-4, Ketoprofen 22204-53-1, Naproxen  
 22494-42-4, Diflunisal 23031-25-6, Terbutaline 23214-92-8, Doxorubicin  
 24219-97-4, Mianserin 25614-03-3, Bromocriptine 26787-78-0,  
 Amoxicillin 26839-75-8, Timolol 28395-03-1, Bumetanide 28911-01-5,  
 Triazolam 28981-97-7, Alprazolam 29094-61-9, Glipizide 29122-68-7,  
 Atenolol 29679-58-1, Fenoprofen 30516-87-1, Zidovudine 31828-71-4,  
 Mexiletine 32795-44-1, N-Acetylprocainamide 32887-01-7, Mecillinam  
 33419-42-0 36507-30-9, Carbamazepine-10,11-epoxide 36894-69-6,  
 Labetalol 37517-30-9, Acebutolol 38304-91-5, Minoxidil 38821-53-3,  
 Cephadrine 41708-72-9, Tocainide 42200-33-9, Nadolol 42399-41-7,  
 Diltiazem 50370-12-2, Cefadroxil 51384-51-1, Metoprolol 51481-61-9,

Cimetidine 54143-55-4, Flecainide 54910-89-3, Fluoxetine 55985-32-5,  
 Nicardipine 56775-88-3, Zimelidine 58001-44-8, Clavulanic acid  
 59277-89-3, Acyclovir 59467-70-8, Midazolam 59865-13-3, Cyclosporine  
 60719-84-8, Amrinone 62571-86-2, Captopril 63590-64-7, Terazosin  
 64952-97-2, Moxalactam 66357-35-5, Ranitidine 66778-36-7, Encainide  
 70458-96-7, Norfloxacin 75847-73-3, Enalapril 76824-35-6, Famotidine  
 76963-41-2, Nizatidine 85721-33-1

RL: BIOL (Biological study)

(non-congeneric structure-pharmacokinetic property  
 correlation of, oral bioavailability simulation with, fuzzy adaptive  
 least squares in)

ACCESSION NUMBER: 1994:400248 HCAPLUS

121:248

TITLE: Non-congeneric structure-pharmacokinetic  
 property correlation studies using fuzzy adaptive  
 least-squares: oral bioavailability

AUTHOR(S): Hirono, Shuichi; Nakagome, Izumi; Hirano, Hiroyuki;  
 Matsushita, Yasuo; Yoshii, Fumiko; Moriguchi, Ikuo

CORPORATE SOURCE: Sch. Pharm. Sci., Kitasato Univ., Tokyo, 108, Japan  
 SOURCE: Biological & Pharmaceutical Bulletin (1994),

17(2), 306-9

CODEN: BPBLEO; ISSN: 0918-6158

DOCUMENT TYPE: Journal

LANGUAGE: English

ABSTRACT:

Quant. relationship between chemical structure and oral bioavailability of 188 non-congeneric organic medicinals were studied to construct an expert system for predicting pharmacokinetic properties of organic chems. The compds. studied were classified into three groups: non-aroms., aroms., and heteroaroms. Their oral bioavailability data observed in human adults were allotted into three ratings, and the relationships with chemical structure were analyzed using fuzzy adaptive least-squares. Quant. relationship models formulated for the three structure groups gave significant information about factors influencing bioavailability, and were statistically reliable in both recognition and leave-one-out prediction despite the diversity and complexity of the structures of the compds. investigated.

=> DIS L17 1 SAM IBIB IABS

THE ESTIMATED COST FOR THIS REQUEST IS 3.07 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L17 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

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IT Simulation and Modeling, biological  
 (of drug oral bioavailability, non-congeneric structure-  
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IT Pharmacokinetics  
 (of drugs, structure and oral bioavailability in relation to)

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IT 50-02-2, Dexamethasone 50-06-6, Phenobarbital, biological studies  
 50-18-0, Cyclophosphamide 50-24-8, Prednisolone 50-33-9,  
 Phenylbutazone, biological studies 50-36-2, Cocaine 50-44-2,  
 Mercaptopurine 50-47-5, Desipramine 50-48-6, Amitriptyline 50-49-7,  
 Imipramine 50-53-3, biological studies 50-78-2, Acetylsalicylic acid

51-06-9, Procainamide 51-21-8, Fluorouracil 51-34-3, Scopolamine  
 51-48-9, L-Thyroxine, biological studies 51-55-8, Atropine,  
 biological studies 52-01-7, Spironolactone 52-53-9, Verapamil  
 52-86-8, Haloperidol 53-03-2 53-86-1, Indomethacin 54-05-7,  
 Chloroquine 54-11-5, Nicotine 54-31-9, Furosemide 55-63-0,  
 Nitroglycerin 56-29-1, Hexobarbital 56-54-2, Quinidine 56-75-7,  
 Chloramphenicol 57-27-2, Morphine, biological studies 57-41-0,  
 Phenytoin 57-42-1, Meperidine 57-66-9, Probenecid 57-96-5,  
 Sulfinpyrazone 58-08-2, Caffeine, biological studies 58-25-3,  
 Chlordiazepoxide 58-55-9, Theophylline, biological studies 58-73-1  
 58-93-5, Hydrochlorothiazide 59-05-2, Methotrexate 59-41-6, Bretylium  
 60-54-8, Tetracycline 61-33-6, Benzylpenicillin, biological studies  
 61-72-3, Cloxacillin 64-17-5, Ethanol, biological studies  
 64-77-7, Tolbutamide 66-79-5, Oxacillin 68-35-9, Sulfadiazine  
 69-53-4, Ampicillin 69-72-7, Salicylic acid, biological studies  
 71-63-6, Digitoxin 72-69-5, Nortriptyline 74-55-5, Ethambutol  
 76-57-3, Codeine 76-99-3, Methadone 77-36-1, Chlorthalidone 77-67-8,  
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 86-54-4, Hydralazine 87-08-1, Phenoxymethypenicillin 87-33-2,  
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 Chlorpropamide 99-66-1, Valproic acid 100-33-4, Pentamidine  
 103-90-2, Acetaminophen 113-92-8 114-07-8, Erythromycin 125-33-7,  
 Primidone 127-69-5, Sulfisoxazole 129-20-4, Oxyphenbutazone  
 130-95-0, Quinine 137-58-6, Lidocaine 146-22-5 147-52-4, Nafcillin  
 147-94-4, Cytarabine 148-82-3, Melphalan 155-97-5, Pyridostigmine  
 298-46-4, Carbamazepine 298-50-0, Propantheline 305-03-3, Chlorambucil  
 315-30-0, Allopurinol 359-83-1, Pentazocine 364-62-5, Metoclopramide  
 364-98-7, Diazoxide 378-44-9, Betamethasone 396-01-0, Triamterene  
 438-60-8, Protriptyline 439-14-5, Diazepam 443-48-1, Metronidazole  
 446-86-6, Azathioprine 465-65-6, Naloxone 525-66-6, Propranolol  
 555-30-6, Methyldopa 564-25-0, Doxycycline 604-75-1 637-07-0,  
 Clofibrate 657-24-9, Metformin 738-70-5, Trimethoprim 768-94-5,  
 Amantadine 846-49-1, Lorazepam 846-50-4, Temazepam 1088-11-5,  
 Desmethyl diazepam 1622-61-3, Clonazepam 1622-62-4, Flunitrazepam  
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 Tetrahydrocannabinol 2022-85-7, Flucytosine 2062-78-4, Pimozide  
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 5250-39-5, Flucloxacillin 6452-71-7, Oxprenolol 6493-05-6,  
 Pentoxyfylline 6740-88-1, Ketamine 6893-02-3, Triiodothyronine  
 7206-76-0, Phenylethylmalonamide 10118-90-8, Minocycline 10262-69-8,  
 Maprotiline 13523-86-9, Pindolol 13655-52-2, Alprenolol 15307-86-5,  
 Diclofenac 15686-71-2, Cephalexin 15687-27-1, Ibuprofen 16051-77-7,  
 Isosorbide-5-mononitrate 16106-20-0, Isosorbide-2-mononitrate  
 16590-41-3, Naltrexone 18323-44-9, Clindamycin 19216-56-9, Prazosin  
 19794-93-5, Trazodone 20594-83-6, Nalbuphine 20830-75-5, Digoxin  
 21829-25-4, Nifedipine 22071-15-4, Ketoprofen 22204-53-1, Naproxen  
 22494-42-4, Diflunisal 23031-25-6, Terbutaline 23214-92-8, Doxorubicin  
 24219-97-4, Mianserin 25614-03-3, Bromocriptine 26787-78-0,  
 Amoxicillin 26839-75-8, Timolol 28395-03-1, Bumetanide 28911-01-5,  
 Triazolam 28981-97-7, Alprazolam 29094-61-9, Glipizide 29122-68-7,  
 Atenolol 29679-58-1, Fenoprofen 30516-87-1, Zidovudine 31828-71-4,  
 Mexiletine 32795-44-1, N-Acetylprocainamide 32887-01-7, Mecillinam  
 33419-42-0 36507-30-9, Carbamazepine-10,11-epoxide 36894-69-6,  
 Labetalol 37517-30-9, Acebutolol 38304-91-5, Minoxidil 38821-53-3,  
 Cephadrine 41708-72-9, Tocainide 42200-33-9, Nadolol 42399-41-7,  
 Diltiazem 50370-12-2, Cefadroxil 51384-51-1, Metoprolol 51481-61-9,  
 Cimetidine 54143-55-4, Flecainide 54910-89-3, Fluoxetine 55985-32-5,  
 Nicardipine 56775-88-3, Zimelidine 58001-44-8, Clavulanic acid  
 59277-89-3, Acyclovir 59467-70-8, Midazolam 59865-13-3, Cyclosporine  
 60719-84-8, Amrinone 62571-86-2, Captopril 63590-64-7, Terazosin  
 64952-97-2, Moxalactam 66357-35-5, Ranitidine 66778-36-7, Encainide  
 70458-96-7, Norfloxacin 75847-73-3, Enalapril 76824-35-6, Famotidine  
 76963-41-2, Nizatidine 85721-33-1

RL: BIOL (Biological study)

(non-congeneric structure-pharmacokinetic property)

correlation of, oral bioavailability simulation with, fuzzy adaptive least squares in)

ACCESSION NUMBER: 1994:400248 HCPLUS

DOCUMENT NUMBER: 121:248

TITLE: Non-congeneric structure-pharmacokinetic property correlation studies using fuzzy adaptive least-squares: oral bioavailability

AUTHOR(S): Hirano, Shuichi; Nakagome, Izumi; Hirano, Hiroyuki; Matsushita, Yasuo; Yoshii, Fumiko; Moriguchi, Ikuo

CORPORATE SOURCE: Sch. Pharm. Sci., Kitasato Univ., Tokyo, 108, Japan

SOURCE: Biological & Pharmaceutical Bulletin (1994), 17(2), 306-9

DOCUMENT TYPE: Journal

LANGUAGE: English

ABSTRACT: Quant. relationship between chemical structure and oral bioavailability of 188 non-congeneric organic medicinals were studied to construct an expert system for predicting pharmacokinetic properties of organic chems. The compds. studied were classified into three groups: non-aroms., aroms., and heteroaroms. Their oral bioavailability data observed in human adults were allotted into three ratings, and the relationships with chemical structure were analyzed using fuzzy adaptive least-squares. Quant. relationship models formulated for the three structure groups gave significant information about factors influencing bioavailability, and were statistically reliable in both recognition and leave-one-out prediction despite the diversity and complexity of the structures of the compds. investigated.

=> FOCUS L17  
 PROCESSING COMPLETED FOR L17  
 L18 9 FOCUS L17 1-

=> DIS L18 1 SAM IBIB IABS

L18 ANSWER 1 OF 9 HCPLUS COPYRIGHT 2006 ACS on STN  
 CC 1-11 (Pharmacology)  
 Section cross-reference(s): 4, 14  
 TI Kinetics of drug action in disease states. XXXIV. Effect of experimental thyroid disorders on the pharmacodynamics of phenobarbital, ethanol and pentylenetetrazol  
 ST thyroid disorder phenobarbital ethanol pentylenetetrazole pharmacol  
 IT Brain, metabolism  
 (ethanol and pentylenetetrazole and phenobarbital metabolism by, thyroid disorder effect on)  
 IT Cerebrospinal fluid  
 (ethanol and pentylenetetrazole and phenobarbital of, thyroid disorder effect on)  
 IT Hyperthyroidism  
 Hypothyroidism  
 (ethanol and pentylenetetrazole and phenobarbital pharmacodynamics response to)  
 IT 50-06-6, Phenobarbital, biological studies 54-95-5, Pentylenetetrazole  
 64-17-5, Ethanol, biological studies  
 RL: BIOL (Biological study)  
 (pharmacodynamics of, thyroid disorder effect on)

ACCESSION NUMBER: 1989:225400 HCPLUS  
 DOCUMENT NUMBER: 110:225400  
 TITLE: Kinetics of drug action in disease states. XXXIV. Effect of experimental thyroid disorders on the pharmacodynamics of phenobarbital, ethanol and pentylenetetrazol  
 AUTHOR(S): Walker, Judith S.; Levy, Gerhard

CORPORATE SOURCE: Sch. Pharm., State Univ. New York, Buffalo, Amherst, NY, 14260, USA  
 SOURCE: Journal of Pharmacology and Experimental Therapeutics (1989), 249(1), 6-10  
 CODEN: JPETAB; ISSN: 0022-3565  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ABSTRACT:

To determine the effect of thyroid disorders on the concentration-activity relationship of title drugs acting on the central nervous system, rats were made hyperthyroid by administration of L-thyroxine and hypothyroid by administration of propylthiouracil. From the results, it is concluded that exptl. thyroid disorders had no pronounced effect on the pharmacodynamics (concentration-effect relationship) of phenobarbital, ethanol and pentylenetetrazol in rats.

=> DIS L18 2 - SAM IBIB IABS  
 YOU HAVE REQUESTED DATA FROM 8 ANSWERS - CONTINUE? Y/ (N) :Y

L18 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN  
 IC ICM A61K045-06  
 ICS A61K031-195; A61K031-135; A61K031-00; A61K037-24  
 CC 63-6 (Pharmaceuticals)  
 Section cross-reference(s): 1  
 TI  $\beta$ -adrenergic agonist and thyroid hormone-containing pharmaceutical composition for treatment of lung obstructions  
 ST lung obstruction terbutaline triiodothyronine; asthma adrenergic agonist thyroid hormone  
 IT Thyroid hormones  
 RL: BIOL (Biological study)  
 (pharmaceuticals containing  $\beta$ -adrenergic agonists and, for lung obstructions)  
 IT Pharmaceutical dosage forms  
 (aerosols,  $\beta$ -adrenergic agonist and thyroid hormone-containing, for lung obstructions)  
 IT Bronchodilators  
 (antiasthmatics,  $\beta$ -adrenergic agonist and thyroid hormone-containing pharmaceutical composition for)  
 IT Pharmaceutical dosage forms  
 (inhalants,  $\beta$ -adrenergic agonist and thyroid hormone-containing, for lung obstructions)  
 IT Pharmaceutical dosage forms  
 (injections,  $\beta$ -adrenergic agonist and thyroid hormone-containing, for lung obstructions)  
 IT Lung, disease or disorder  
 (obstruction, treatment of,  $\beta$ -adrenergic agonist and thyroid hormone-containing pharmaceutical composition for)  
 IT Pharmaceutical dosage forms  
 (oral,  $\beta$ -adrenergic agonist and thyroid hormone-containing, for lung obstructions)  
 IT Pharmaceutical dosage forms  
 (powders,  $\beta$ -adrenergic agonist and thyroid hormone-containing, for lung obstructions)  
 IT Adrenergic agonists  
 ( $\beta$ -, pharmaceuticals containing thyroid hormones and, for lung obstructions)  
 IT 51-43-4, Epinephrine 586-06-1, Orciprenaline 7683-59-2, Isoprenaline 13392-18-2 18559-94-9 23031-25-6, Terbutaline 23031-32-5, Terbutalin sulfate 32953-89-2  
 RL: BIOL (Biological study)  
 (as  $\beta$ -adrenergic agonist, pharmaceutical containing thyroid hormones and, for lung obstructions)  
 IT 51-48-9, Thyroxine, biological studies 1041-01-6,

Diodothyronine 6893-02-3, Triiodothyronine  
 RL: BIOL (Biological study)  
 (pharmaceutical composition containing  $\beta$ -adrenergic agonist and,  
 for lung obstructions)  
 ACCESSION NUMBER: 1990:185806 HCPLUS  
 DOCUMENT NUMBER: 112:185806  
 TITLE:  $\beta$ -adrenergic agonist and thyroid  
 hormone-containing pharmaceutical  
 composition for treatment of lung obstructions  
 INVENTOR(S): Smith, Ulf Per Gustav; Wesslau, Christian  
 PATENT ASSIGNEE(S): Swed.  
 SOURCE: PCT Int. Appl., 9 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8907454	A1	19890824	WO 1989-SE57	19890210 <--
W: DK, FI, JP, NO, US				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
SE 8800461	A	19890812	SE 1988-461	19880211 <--
SE 461013	B	19891218		
SE 461013	C	19900412		
EP 357725	A1	19900314	EP 1989-902559	19890210 <--
EP 357725	B1	19920415		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
JP 03500294	T2	19910124	JP 1989-502359	19890210 <--
AT 74767	E	19920515	AT 1989-902559	19890210 <--
NO 8904030	A	19891009	NO 1989-4030	19891009 <--
DK 8905005	A	19891010	DK 1989-5005	19891010 <--
PRIORITY APPLN. INFO.:			SE 1988-461	A 19880211
			EP 1989-902559	A 19890210
			WO 1989-SE57	W 19890210

## ABSTRACT:

A pharmaceutical composition for therapeutic and/or prophylactic treatment of lung obstructions consists of a therapeutically active amount of  $\beta$ -adrenergic agonist and that of active thyroid hormones (preferred ratio 10:1-1:1). Thus, terbutaline sulfate and triiodothyronine were granulated with \*\*\*ethanol\*\*\* /water containing 1-2% of sorbitan, dried, and then ground to a fine powder having a particle size suitable for being administered in the form of an inhalation aerosol for the local treatment of the lungs. The molar ratio of terbutaline:triiodothyronine was 50:50. The preparation is therapeutic as well as prophylactic treatment for asthma patients.

L18 ANSWER 3 OF 9 HCPLUS COPYRIGHT 2006 ACS on STN  
 CC 58 (Hormones)  
 TI Interaction of ethanol and thyroxine on mitochondria  
 IT Mitochondria  
 (effect of ETOH and thyroxine on)  
 IT 64-17-5, Ethyl alcohol  
 (mitochondrial response to thyroxine and)  
 IT 51-48-9, Thyroxine  
 (mitochondrial response to, ethyl alc. effect on)  
 ACCESSION NUMBER: 1965:418203 HCPLUS  
 DOCUMENT NUMBER: 63:18203  
 ORIGINAL REFERENCE NO.: 63:3261a-c  
 TITLE: Interaction of ethanol and thyroxine  
 on mitochondria  
 AUTHOR(S): Karler, Ralph; Sulkowski, Thomas S.; Miyahara, James T.  
 CORPORATE SOURCE: Dept. of Pharmacol., Univ. of Utah, Coll. of Med.,

SOURCE: Salt Lake City  
 Biochemical Pharmacology (1965), 14 (6),  
 1025-35  
 CODEN: BCPCA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ABSTRACT:

Thyroxine can stimulate mitochondrial swelling and uncoupled oxidative phosphorylation. It was observed that EtOH inhibits both spontaneous and thyroxine-induced mitochondrial swelling. The antiswelling activity of EtOH is manifested during mitochondrial respiration both in the presence and absence of phosphorylation. EtOH was observed only to block \*\*\*thyroxine\*\*\* -induced swelling; it could not reverse the swelling. EtOH also blocked Ca++ and phosphate-induced swelling. Therefore, the antiswelling activity of EtOH is more generalized than that of serum albumin. It is concluded that the EtOH antagonism of mitochondrial swelling produced by various agents is probably dependent on the fact that EtOH alone inhibits swelling; EtOH is therefore a pharmacol. antagonist of agents that induce swelling. In addition to inhibiting swelling, EtOH also blocks uncoupling of oxidative phosphorylation by thyroxine and Ca++ but not by salicylate. These observations were interpreted to indicate that EtOH affects oxidative phosphorylation only indirectly by blocking mitochondrial swelling. The observed effects of EtOH on mitochondria are discussed in terms of reports on the ability of thyroid hormone to antagonize acute alc. intoxication in man, and the ability of EtOH to block effects of Ca++ on smooth muscle.

L18 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN  
 IC ICM A61L015-16  
 INCL 424447000  
 CC 63-6 (Pharmaceuticals)  
 TI Controlled-release transdermal pharmaceuticals containing cryogels  
 ST controlled release transdermal pharmaceutical cryogel; ciprofloxacin polyvinyl alc cryogel transdermal pharmaceutical  
 IT Vitamins  
 RL: BIOL (Biological study)  
 (J, controlled-release transdermal pharmaceuticals containing cryogels and)  
 IT Manganins (proteins)  
 Thyroglobulins  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (controlled-release transdermal pharmaceuticals containing cryogels and)  
 IT Quaternary ammonium compounds, biological studies  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (alkylbenzyldimethyl, chlorides, controlled-release transdermal pharmaceuticals containing cryogels and)  
 IT Animal growth regulators  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (blood platelet-derived growth factors, controlled-release transdermal pharmaceuticals containing cryogels and)  
 IT Agglutinins and Lectins  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (cecropins, controlled-release transdermal pharmaceuticals containing cryogels and)  
 IT Gels  
 (cryogenic, controlled-release transdermal pharmaceuticals 60contg. therapeutic agents and)  
 IT Pharmaceutical natural products  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (digitalis, controlled-release transdermal pharmaceuticals containing cryogels and)  
 IT Animal growth regulators  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(epithelium-derived growth factors, controlled-release transdermal pharmaceuticals containing cryogels and)

IT Fatty acids, biological studies

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(essential, controlled-release transdermal pharmaceuticals containing cryogels and)

IT Pharmaceutical dosage forms

(transdermal, controlled-release, cryogels and therapeutic agents in)

IT 50-00-0, Formaldehyde, biological studies 50-02-2, Dexamethasone  
50-06-6, biological studies 50-07-7, Mitomycin C 50-18-0, Cytoxan  
50-23-7, Hydrocortisone 50-24-8, Prednisolone 50-48-6, Amitriptyline  
50-49-7, Imipramine 50-52-2, Thioridazine 50-53-3, Chlorpromazine,  
biological studies 50-56-6, Oxytocin, biological studies 50-76-0,  
Actinomycin D 50-78-2 50-81-7, Vitamin C, biological studies  
51-05-8, Procaine hydrochloride 51-21-8, 5-Fluorouracil 51-34-3,  
Scopolamine 51-41-2, Levarterenol 51-43-4, Epinephrine 51-48-9,  
Thyroxine, biological studies 51-64-9, Dextroamphetamine  
51-77-4, Gefarnate 52-53-9, Verapamil 52-86-8, Haloperidol 53-03-2,  
Prednisone 53-06-5, Cortisone 54-31-9, Furosemide 54-42-2,  
Idoxuridine 54-85-3, Isoniazide 54-91-1, Pipobroman 55-63-0  
56-40-6, Glycine, biological studies 56-41-7, Alanine, biological  
studies 56-45-1, Serine, biological studies 56-54-2, Quinidine  
56-75-7, Chloramphenicol 56-84-8, Aspartic acid, biological studies  
56-85-9, Glutamine, biological studies 56-86-0, Glutamic acid,  
biological studies 56-87-1, Lysine, biological studies 57-27-2,  
Morphine, biological studies 57-41-0, Phenytoin 57-42-1, Meperidine  
57-66-9, Probenecid 57-92-1, Streptomycin, biological studies 58-08-2,  
biological studies 58-14-0, Pyrimethamine 58-32-2, Dipyridamole  
58-40-2, Promazine 58-54-8, Ethacrynic acid 58-55-9, Theophylline,  
biological studies 58-73-1, Diphenhydramine 58-74-2, Papaverine  
58-93-5 59-01-8, Kanamycin 59-05-2, Methotrexate 59-33-6 59-46-1,  
Procaine 59-87-0 59-92-7, Levodopa, biological studies 60-54-8,  
Tetracycline 61-25-6, Papaverine hydrochloride 61-32-5, Methicillin  
61-33-6, preparation 61-72-3, Cloxacillin 61-90-5, L-Leucine,  
biological studies 62-31-7, Dopamine hydrochloride 62-97-5, Diphenamid  
63-68-3, Methionine, biological studies 63-91-2, Phenylalanine,  
biological studies 64-17-5, Ethanol, biological studies  
65-49-6 66-79-5, Oxacillin 67-63-0, Isopropanol, biological studies  
68-88-2, Hydroxyzine 69-23-8, Fluphenazine 69-43-2, Prenylamine  
lactate 69-53-4, Ampicillin 69-72-7, biological studies 70-00-8,  
Trifluridine 70-30-4, Hexachlorophene 71-00-1, Histidine, biological  
studies 72-19-5, Threonine, biological studies 72-44-6, Methaqualone  
72-69-5 73-22-3, Tryptophan, biological studies 73-32-5, Isoleucine,  
biological studies 73-48-3 74-79-3, Arginine, biological studies  
76-99-3, Methadone 77-07-6, Levorphanol 77-19-0, Dicyclomine  
77-21-4, Glutethimide 78-11-5, Pentaerythritol tetranitrate 79-57-2,  
Oxytetracycline 81-23-2, Dehydrocholic acid 83-88-5, Vitamin G,  
biological studies 83-98-7, Orphenadrine 85-79-0, Dibucaine 86-21-5,  
Pheniramine 86-22-6, Brompheniramine 87-08-1, Penicillin V 87-33-2,  
Isosorbide dinitrate 90-82-4, Pseudoephedrine 91-81-6, Tripelennamine  
94-09-7, Benzocaine 95-27-2, Dimazole 100-92-5, Mephentermine  
101-31-5, Hyoscyamine 108-46-3, 1,3-Benzenediol, biological studies  
112-38-9, Undecylenic acid 113-15-5, Ergotamine 113-92-8 114-07-8,  
Erythromycin 115-38-8, Methylphenobarbital 118-23-0,  
Bromodiphenhydramine 118-42-3, Hydroxychloroquine 121-54-0 122-09-8,  
Phentermine 122-11-2, Sulfadimethoxine 125-29-1, Hydrocodone  
125-71-3, Dextromethorphan 126-07-8, Griseofulvin 127-33-3,  
Demeclocycline 127-69-5, Sulfisoxazole 128-62-1, Noscapine 129-16-8,  
Mercurochrome 132-17-2 133-15-3 133-67-5, Trichlormethiazide  
136-96-9 137-58-6, Lidocaine 144-80-9, Sulfacetamide 144-82-1,  
Sulfamethizole 147-24-0, Diphenhydramine hydrochloride 147-52-4,  
Naftillin 147-85-3, Proline, biological studies 148-82-3, Melphalan  
151-21-3, Sodium lauryl sulfate, biological studies 153-61-7,  
Cephalothin 154-21-2 298-57-7, Cinnarizine 300-62-9, Amphetamine  
302-17-0, Chloral hydrate 302-79-4, Retinoic acid 303-81-1, Novobiocin

303-98-0 318-98-9 359-83-1, Pentazocine 361-37-5, Methysergide  
 389-08-2, Nalidixic acid 395-28-8, Isoxsuprime 437-38-7, Fentanyl  
 439-14-5, Diazepam 447-41-6 466-99-9, Hydromorphone 469-62-5,  
 Propoxyphene 471-53-4, Glycyrrhetic acid 479-18-5, Diprophylline  
 486-12-4, Triprolidine 496-67-3, Bromovalerylurea 514-65-8, Biperiden  
 515-64-0, Sulfisomidine 525-66-6, Propranolol 554-13-2, Lithium  
 carbonate 562-10-7 564-25-0, Doxycycline 569-65-3, Meclizine  
 634-03-7, Phendimetrazine 645-05-6, HMM 668-94-0 671-16-9,  
 Procarbazine 770-05-8, Octopamine hydrochloride 777-11-7, Haloprogin  
 804-10-4 807-38-5, Fluocinolone 835-31-4, Naphazoline 914-00-1,  
 Methacycline 940-69-2, Vitamin N 1018-71-9, Pyrrolnitrin 1066-17-7,  
 Colistin 1070-11-7 1115-84-0, Vitamin U 1172-18-5, Flurazepam  
 hydrochloride 1319-77-3, Cresol 1319-82-0, Aminocaproic acid  
 1333-08-0, Ethyl aminobenzoate 1333-73-9, Sodium borate 1340-08-5,  
 Vitamin P 1394-02-1, Trichomycin 1397-89-3, Amphotericin B  
 1400-61-9, Nystatin 1403-66-3, Gentamicin 1404-00-8, Mitomycin  
 1404-04-2, Neomycin 1404-90-6, Vancomycin 1405-87-4, Bacitracin  
 1405-97-6, Gramicidin 1406-11-7, Polymyxin 1406-16-2, Vitamin D  
 1406-18-4, Vitamin E 1407-73-4, Vitamin T 1538-09-6 1668-19-5,  
 Doxepin 1695-77-8, Spectinomycin 1766-91-2, Penflutizide 1982-36-1,  
 Homochlorcyclizine hydrochloride 1982-37-2, Methdilazine 2011-67-8,  
 Nimetazepam 2013-58-3, Meclocycline 2020-25-9 2022-85-7, Flucytosine  
 2338-37-6, Levoproxyphene 2398-96-1, Tolnaftate 2751-09-9,  
 Troleandomycin 2751-68-0 3116-76-5, Dicloxacillin 3485-14-1  
 3562-84-3, Benzboromarone 3737-09-5, Disopyramide 3922-90-5,  
 Oleandomycin 4205-90-7, Clonidine 4299-60-9, Sulfisoxazole diolamine  
 4342-03-4, DTIC 4697-36-3, Carbenicillin 5536-17-4, Vidarabine  
 5588-33-0, Mesoridazine 6452-73-9, Oxprenolol hydrochloride 6493-05-6,  
 Pentoxyfylline 6834-98-6, Pentamycin 7195-27-9, Mefruside 7237-81-2,  
 Hepronicate 7440-22-4D, Silver, salts 7440-45-1D, Cerium, salts  
 7440-66-6D, Zinc, salts 7487-94-7, Mercuric chloride, biological studies  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (controlled-release transdermal pharmaceuticals containing  
 cryogels and)

IT 7542-37-2 7722-64-7, Potassium permanganate 8017-57-0,  
 Trisulfapyrimidine 8049-47-6, Pancreatin 9001-09-6, Chymopapain  
 9001-12-1, Collagenase 9001-73-4, Papain 9001-75-6, Pepsin  
 9001-90-5, Fibrinolysin 9001-98-3, Rennin 9002-01-1, Streptokinase  
 9002-07-7, Trypsin 9002-60-2, ACTH, biological studies 9002-64-6,  
 Parathyrin 9002-71-5, Thyrotropin 9002-72-6, Somatotropin 9003-98-9,  
 Desoxyribonuclease 9004-07-3, Chymotrypsin 9004-10-8, Insulin,  
 biological studies 9005-49-6, Heparin, biological studies 9007-12-9,  
 Calcitonin 9015-68-3, Asparaginase 9039-53-6, Urokinase 10043-35-3,  
 Boric acid, biological studies 10118-90-8, Minocycline 10262-69-8,  
 Maprotiline 10540-29-1, Tamoxifen 11000-17-2, Vasopressin  
 11011-73-7, Bramycin 11056-06-7, Bleomycin 11103-57-4, Vitamin A  
 11111-12-9, Cephalosporin 12001-76-2, Vitamin B 12001-79-5, Vitamin K  
 12211-28-8, Sutilains 12607-92-0, Aceglutamide aluminum 12629-01-5,  
 Somatropin 13010-47-4, CCNU 13171-25-0 13265-10-6, Methscopolamine  
 13292-46-1, Rifampin 13523-86-9, Pindolol 14838-15-4,  
 Phenylpropanolamine 14929-11-4, Simfibrate 15148-80-8, Bupranolol  
 hydrochloride 15307-86-5, Diclofenac 15421-84-8, Trapidil  
 15663-27-1, cis-Platinum 15686-71-2, Cephalexin 15687-27-1, Ibuprofen  
 16051-77-7, Isosorbide-5-mononitrate 16110-51-3, Cromolyn 17617-23-1,  
 Flurazepam 17902-23-7, Tegafur 18323-44-9, Clindamycin 18378-89-7,  
 Plicamycin 18472-51-0, Chlorhexidine gluconate 19237-84-4, Prazosin  
 hydrochloride 19504-77-9, Variotin 20153-98-4, Dilazep dihydrochloride  
 20830-75-5, Digoxin 20830-81-3, Daunorubicin 21593-23-7, Cephapirin  
 21829-25-4 22071-15-4, Ketoprofen 22161-81-5, S-Ketoprofen  
 22199-08-2, Silver sulfadiazine 22204-53-1 22494-42-4, Diflunisal  
 22733-60-4, Siccanin 22916-47-8 23210-58-4, Ifenprodil tartrate  
 23214-92-8, Doxorubicin 23593-75-1, Clotrimazole 25523-97-1,  
 Dexchlorpheniramine 25655-41-8, Povidone iodine 25717-80-0,  
 Molsidomine 25812-30-0, Gemfibrozil 25953-19-9, Cefazolin  
 25990-43-6, Mepenzolate 26328-04-1, Cinepazide maleate 26787-78-0,

Amoxicillin 27060-91-9, Flutazolam 27164-43-8 27321-61-5,  
 1,2,3-Propanetriolmononitrate 27724-96-5, Cetraxate hydrochloride  
 27959-26-8, Nicomol 28058-62-0 28088-64-4 28395-03-1 28657-80-9,  
 Cinoxacin 28911-01-5 29122-68-7, Atenolol 29679-58-1, Fenoprofen  
 29868-97-1, Pirenzepine hydrochloride 29975-16-4, Estazolam  
 30516-87-1, AZT 30685-43-9, Metildigoxin 32887-01-7, Amdinocillin  
 33069-62-4, Taxol 33286-22-5, Diltiazem hydrochloride 33419-42-0, VP16  
 33665-90-6 33671-46-4, Clotiazepam 34444-01-4, Cefamandole  
 34580-13-7, Ketotifen 34787-01-4 34915-68-9, Bunitrolol 35607-66-0,  
 Cefoxitin 37091-66-0, Azlocillin 37517-28-5, Amikacin 38194-50-2,  
 Sulindac 38821-53-3, Cephadrine 49745-95-1, Dobutamine hydrochloride  
 50370-12-2, Cefadroxil 50972-17-3, Bacampicillin 51384-51-1,  
 Metoprolol 51481-61-9, Cimetidine 51481-65-3, Mezlocillin  
 51781-21-6, Carteolol hydrochloride 51940-44-4, Pipemidic acid  
 53608-75-6, Pancrelipase 53902-12-8, Tranilast 53994-73-3, Cefaclor  
 54527-84-3, Nicardipine hydrochloride 55268-75-2, Cefuroxime  
 55985-32-5, Nicardipine 56391-56-1, Netilmicin 56392-17-7, Metoprolol  
 tartrate 58001-44-8 59128-97-1, Haloxazolam 59277-89-3, Acyclovir  
 60925-61-3, Ceforanide 61270-58-4, Cefonicid 61422-45-5, Carmofur  
 61477-96-1, Piperacillin 62229-50-9, Epidermal growth factor  
 62683-29-8, CSF 62893-19-0, Cefoperazone 63527-52-6, Cefotaxime  
 64221-86-9, Imipenem 64952-97-2, Moxalactam 66676-88-8, Aclacinomycin  
 67763-96-6, IGF-1 68247-85-8, Peplomycin 68401-81-0, Ceftizoxime  
 70458-92-3 70458-96-7, Norfloxacin 72558-82-8, Ceftazidime  
 73384-59-5, Ceftriaxone 74011-58-8, Enoxacin 78186-34-2, Bisantrene  
 79217-60-0, Cyclosporin 79660-72-3, Fleroxacin 82009-34-5, Cilastatin  
 82030-87-3, Somatrem 82410-32-0, Gancyclovir 82419-36-1, Ofloxacin  
 82657-92-9, Pro-urokinase 83869-56-1, Colony-stimulating factor 2  
 84137-20-2, 1,2,3-Propanetriolnitrate 85721-33-1, Ciprofloxacin  
 98079-51-7, Lomefloxacin 100490-36-6 105636-15-5, Suprasec VM 25  
 118857-69-5D, alkyl derivs. 135968-09-1, RG-CSF 139639-23-9  
 150977-36-9, Bromelain

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (controlled-release transdermal pharmaceuticals containing  
 cryogels and)

ACCESSION NUMBER: 1994:200438 HCAPLUS  
 DOCUMENT NUMBER: 120:200438  
 TITLE: Controlled-release transdermal pharmaceuticals  
 containing cryogels  
 INVENTOR(S): Wood, Louis L.; Calton, Gary J.  
 PATENT ASSIGNEE(S): SRCHEM Inc., USA  
 SOURCE: U.S., 15 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5260066	A	19931109	US 1992-821627	19920116 <--
US 5288503	A	19940222	US 1992-899369	19920616 <--
PRIORITY APPLN. INFO.:			US 1992-821627	A3 19920116

ABSTRACT:

A controlled-release transdermal pharmaceutical containing therapeutic agents in a poly(vinyl alc.) (I) cryogel is disclosed. A slurry of 11.0 mg ciprofloxacin.HCl (II) and 200 mg 10% I was warmed to 50-60° to obtain a clear homogeneous solution. The solution was then placed in a mold and subjected to 6 freeze-thaw cycles to give a white opaque elastomeric cryogel having 15mm diameter and 0.5mm thickness. The release of II from the gel in 0.9% NaCl was 74% in the 1st 4 hs and it was constant in the subsequent 5-24 hs.

TI Non-congeneric structure-pharmacokinetic property correlation  
 studies using fuzzy adaptive least-squares: oral bioavailability  
 ST structure pharmacokinetic correlation bioavailability simulation  
 IT Quantitative structure-activity relationship  
     (in drug oral bioavailability simulation)  
 IT Simulation and Modeling, biological  
     (of drug oral bioavailability, non-congeneric structure-  
         pharmacokinetic property correlation in)  
 IT Pharmacokinetics  
     (of drugs, structure and oral bioavailability in relation to)  
 IT Drug bioavailability  
     (simulation of oral, non-congeneric structure-pharmacokinetic  
         property correlation in)  
 IT Molecular structure-biological activity relationship  
     (pharmacokinetic, in drug oral bioavailability simulation)  
 IT 50-02-2, Dexamethasone 50-06-6, Phenobarbital, biological studies  
 50-18-0, Cyclophosphamide 50-24-8, Prednisolone 50-33-9,  
 Phenylbutazone, biological studies 50-36-2, Cocaine 50-44-2,  
 Mercaptopurine 50-47-5, Desipramine 50-48-6, Amitriptyline 50-49-7,  
 Imipramine 50-53-3, biological studies 50-78-2, Acetylsalicylic acid  
 51-06-9, Procainamide 51-21-8, Fluorouracil 51-34-3, Scopolamine  
 51-48-9, L-Thyroxine, biological studies 51-55-8, Atropine,  
 biological studies 52-01-7, Spironolactone 52-53-9, Verapamil  
 52-86-8, Haloperidol 53-03-2 53-86-1, Indomethacin 54-05-7,  
 Chloroquine 54-11-5, Nicotine 54-31-9, Furosemide 55-63-0,  
 Nitroglycerin 56-29-1, Hexobarbital 56-54-2, Quinidine 56-75-7,  
 Chloramphenicol 57-27-2, Morphine, biological studies 57-41-0,  
 Phenytoin 57-42-1, Meperidine 57-66-9, Probenecid 57-96-5,  
 Sulfinpyrazone 58-08-2, Caffeine, biological studies 58-25-3,  
 Chlordiazepoxide 58-55-9, Theophylline, biological studies 58-73-1  
 58-93-5, Hydrochlorothiazide 59-05-2, Methotrexate 59-41-6, Bretylium  
 60-54-8, Tetracycline 61-33-6, Benzylpenicillin, biological studies  
 61-72-3, Cloxacillin 64-17-5, Ethanol, biological studies  
 64-77-7, Tolbutamide 66-79-5, Oxacillin 68-35-9, Sulfadiazine  
 69-53-4, Ampicillin 69-72-7, Salicylic acid, biological studies  
 71-63-6, Digitoxin 72-69-5, Nortriptyline 74-55-5, Ethambutol  
 76-57-3, Codeine 76-99-3, Methadone 77-36-1, Chlorthalidone 77-67-8,  
 Ethosuximide 80-08-0 81-81-2, Warfarin 83-43-2, Methylprednisolone  
 86-54-4, Hydralazine 87-08-1, Phenoxymethylenicillin 87-33-2,  
 Isosorbide dinitrate 90-89-1, Diethylcarbamazine 94-20-2,  
 Chlorpropamide 99-66-1, Valproic acid 100-33-4, Pentamidine  
 103-90-2, Acetaminophen 113-92-8 114-07-8, Erythromycin 125-33-7,  
 Primidone 127-69-5, Sulfisoxazole 129-20-4, Oxyphenbutazone  
 130-95-0, Quinine 137-58-6, Lidocaine 146-22-5 147-52-4, Nafcillin  
 147-94-4, Cytarabine 148-82-3, Melphalan 155-97-5, Pyridostigmine  
 298-46-4, Carbamazepine 298-50-0, Propantheline 305-03-3, Chlorambucil  
 315-30-0, Allopurinol 359-83-1, Pentazocine 364-62-5, Metoclopramide  
 364-98-7, Diazoxide 378-44-9, Betamethasone 396-01-0, Triamterene  
 438-60-8, Protriptyline 439-14-5, Diazepam 443-48-1, Metronidazole  
 446-86-6, Azathioprine 465-65-6, Naloxone 525-66-6, Propranolol  
 555-30-6, Methyldopa 564-25-0, Doxycycline 604-75-1 637-07-0,  
 Clofibrate 657-24-9, Metformin 738-70-5, Trimethoprim 768-94-5,  
 Amantadine 846-49-1, Lorazepam 846-50-4, Temazepam 1088-11-5,  
 Desmethyldiazepam 1622-61-3, Clonazepam 1622-62-4, Flunitrazepam  
 1668-19-5, Doxepin 1951-25-3, Amiodarone 1972-08-3,  
 Tetrahydrocannabinol 2022-85-7, Flucytosine 2062-78-4, Pimozide  
 3116-76-5, Dicloxacillin 3737-09-5, Disopyramide 4205-90-7, Clonidine  
 5250-39-5, Flucloxacillin 6452-71-7, Oxprenolol 6493-05-6,  
 Pentoxyfylline 6740-88-1, Ketamine 6893-02-3, Triiodothyronine  
 7206-76-0, Phenylethylmalonamide 10118-90-8, Minocycline 10262-69-8,  
 Maprotiline 13523-86-9, Pindolol 13655-52-2, Alprenolol 15307-86-5,  
 Diclofenac 15686-71-2, Cephalexin 15687-27-1, Ibuprofen 16051-77-7,  
 Isosorbide-5-mononitrate 16106-20-0, Isosorbide-2-mononitrate  
 16590-41-3, Naltrexone 18323-44-9, Clindamycin 19216-56-9, Prazosin  
 19794-93-5, Trazodone 20594-83-6, Nalbuphine 20830-75-5, Digoxin

21829-25-4, Nifedipine 22071-15-4, Ketoprofen 22204-53-1, Naproxen  
 22494-42-4, Diflunisal 23031-25-6, Terbutaline 23214-92-8, Doxorubicin  
 24219-97-4, Mianserin 25614-03-3, Bromocriptine 26787-78-0,  
 Amoxicillin 26839-75-8, Timolol 28395-03-1, Bumetanide 28911-01-5,  
 Triazolam 28981-97-7, Alprazolam 29094-61-9, Glipizide 29122-68-7,  
 Atenolol 29679-58-1, Fenoprofen 30516-87-1, Zidovudine 31828-71-4,  
 Mexiletine 32795-44-1, N-Acetylprocainamide 32887-01-7, Mecillinam  
 33419-42-0 36507-30-9, Carbamazepine-10,11-epoxide 36894-69-6,  
 Labetalol 37517-30-9, Acebutolol 38304-91-5, Minoxidil 38821-53-3,  
 Cephadrine 41708-72-9, Tocainide 42200-33-9, Nadolol 42399-41-7,  
 Diltiazem 50370-12-2, Cefadroxil 51384-51-1, Metoprolol 51481-61-9,  
 Cimetidine 54143-55-4, Flecainide 54910-89-3, Fluoxetine 55985-32-5,  
 Nicardipine 56775-88-3, Zimelidine 58001-44-8, Clavulanic acid  
 59277-89-3, Acyclovir 59467-70-8, Midazolam 59865-13-3, Cyclosporine  
 60719-84-8, Amrinone 62571-86-2, Captopril 63590-64-7, Terazosin  
 64952-97-2, Moxalactam 66357-35-5, Ranitidine 66778-36-7, Encainide  
 70458-96-7, Norfloxacin 75847-73-3, Enalapril 76824-35-6, Famotidine  
 76963-41-2, Nizatidine 85721-33-1

RL: BIOL (Biological study)

(non-congeneric structure-pharmacokinetic property  
 correlation of, oral bioavailability simulation with, fuzzy adaptive  
 least squares in)

ACCESSION NUMBER: 1994:400248 HCPLUS

DOCUMENT NUMBER: 121:248

TITLE: Non-congeneric structure-pharmacokinetic  
 property correlation studies using fuzzy adaptive  
 least-squares: oral bioavailability

AUTHOR(S): Hirono, Shuichi; Nakagome, Izumi; Hirano, Hiroyuki;

Matsushita, Yasuo; Yoshii, Fumiko; Moriguchi, Ikuo

CORPORATE SOURCE: Sch. Pharm. Sci., Kitasato Univ., Tokyo, 108, Japan

SOURCE: Biological & Pharmaceutical Bulletin (1994),  
 17(2), 306-9

CODEN: BPBLEO; ISSN: 0918-6158

DOCUMENT TYPE: Journal

LANGUAGE: English

ABSTRACT:

Quant. relationship between chemical structure and oral bioavailability of 188 non-congeneric organic medicinals were studied to construct an expert system for predicting pharmacokinetic properties of organic chems. The compds. studied were classified into three groups: non-aroms., aroms., and heteroaroms. Their oral bioavailability data observed in human adults were allotted into three ratings, and the relationships with chemical structure were analyzed using fuzzy adaptive least-squares. Quant. relationship models formulated for the three structure groups gave significant information about factors influencing bioavailability, and were statistically reliable in both recognition and leave-one-out prediction despite the diversity and complexity of the structures of the compds. investigated.

L18 ANSWER 6 OF 9 HCPLUS COPYRIGHT 2006 ACS on STN

CC 11H (Biological Chemistry: Pharmacology)

TI Effect on the electroencephalogram of pharmacodynamic substances  
 of clinical interest

IT Bromides

Nitrogen mustards

Sulfonamides

(effect on brain)

IT Brain

(elec. activity of, drug effect on)

IT Pituitary extracts

(of posterior lobe, brain response to)

IT 51-43-4, Adrenaline 51-45-6, Histamine 51-84-3, Choline, acetyl-  
 54-05-7, Quinoline, 7-chloro-4-(4-diethylamino-1-methylbutylamino)-  
 56-54-2, Quinidine 57-24-9, Strychnine 57-56-7, Semicarbazide  
 57-92-1, Streptomycin 58-73-1, Diphenhydramine 64-85-7,

Corticosterone, deoxy- 130-95-0, Quinine 149-13-3, Procaine, borate  
 9004-10-8, Insulin  
 (brain response to)  
 IT 59-99-4, Neostigmine  
 (brain stimulation by)  
 IT 50-36-2, Cocaine  
 (effect of, on brain)  
 IT 57-27-2, Morphine  
 (effect on body and skin temps. of dog and rat, thermal stimulus  
 response after)  
 IT 50-37-3, Lysergamide, N,N-diethyl- 51-34-3, Scopolamine 51-48-9,  
 Thyroxine 53-06-5, Cortisone 54-04-6, Mescaline 54-85-3,  
 Isoniazid 54-92-2, Iproniazid 54-95-5, Metrazole 55-63-0,  
 Nitroglycerin 55-91-4, Isopropyl phosphorofluoride, (iso-PrO)2FPO  
 56-86-0, Glutamic acid 58-08-2, Caffeine 58-15-1, Aminopyrine  
 58-55-9, Theophylline 59-26-7, Nikethamide 59-43-8, Vitamin, B1  
 59-67-6, Nicotinic acid 60-26-4, Ammonium, hexamethylenebis(trimethyl-  
 64-17-5, Ethyl alcohol 76-22-2, Camphor 76-99-3, Methadone 83-88-5,  
 Vitamin, B2 83-89-6, Quinacrine 90-69-7, Lobeline 95-05-6, Sulfide,  
 bis(diethylthiocarbamoyl) 97-77-8, Disulfide, bis(diethylthiocarbamoyl)  
 101-31-5, Hyoscyamine 107-49-3, Ethyl pyrophosphate, Et4P2O7 124-87-8,  
 Picrotoxin 144-11-6, 1-Piperidinepropanol,  $\alpha$ -cyclohexyl- $\alpha$ -  
 phenyl- 298-45-3, Bulbocapnine 300-62-9, Phenethylamine,  
 $\alpha$ -methyl- 317-34-0, Aminophylline 1406-05-9, Penicillins  
 7439-95-4, Magnesium 7440-09-7, Potassium 7440-23-5, Sodium  
 7440-70-2, Calcium 8059-24-3, Vitamin, B6 8067-24-1, Hydergin  
 9002-60-2, Corticotropin 14798-03-9, Ammonium 15879-93-3, Chloralose  
 (effect on brain)  
 IT 75-87-6, Chloral  
 (effect on electroencephalograms)  
 IT 66-40-0, Ammonium, tetraethyl-  
 (salts, effect on brain)

ACCESSION NUMBER: 1955:85831 HCAPLUS

DOCUMENT NUMBER: 49:85831

ORIGINAL REFERENCE NO.: 49:16205i,16206a-b

TITLE: Effect on the electroencephalogram of  
 pharmacodynamic substances of clinical  
 interest

AUTHOR(S): Verdeaux, G.; Marty, R.

CORPORATE SOURCE: Fac. med., Paris

SOURCE: Revue Neurologique (1954), 91, 405-27

CODEN: RENEAM; ISSN: 0035-3787

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

ABSTRACT:

cf. Toman and Davis, C.A. 44, 3145i. The following substances were assessed for their effect on the electroencephalogram or the electrocorticogram: bromides, chloral hydrate, hyoscine, chloralose, amphetamine, strychnine, glutamic acid, pentamethylethylenetetrazole, insulin, acetylcholine, mescaline, diethylamide of lysergic acid, bulbocapnine, morphine, methadone, cocaine, procaine, adrenaline, eserine, prostigmine, diisopropyl fluorophosphate, tetraethyl pyrophosphate, quaternary ammoniums, hyoscyamine, Artane, diethylnicotinamide, camphor, various xanthines, lobeline, Hydergin, nicotinic acid, nitroglycerin, histamine, diphenyldramamine, ACTH, cortisone, deoxycorticosterone, posterior pituitary extract, thyroxine, various sulfonamides, various antibiotics, semicarbazide, isoniazid, iproniazid, aminophenazone, quinine, quinidine, chloroquine, quinacrine, ethanol, tetraethylthiuram, vitamins B1, B2, and B6, K, Ca, Na, NH4, Mg, picrotoxin, nitrogen mustards. The authors propose five possible classifications for these drugs on the basis of the pharmacology, physiology, electroencephalographic changes, mode of action, and site of action. They propose that the pharmacological effects are either direct on the cell proper, or on an aggregate of cells, or indirect through the modification of the general environment of the cell or the cell aggregates.

L18 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN  
 CC 60 (Biochemical Methods)  
 TI Protozoan assays for vitamins, and cytotoxicity of carcinogens, and pharmacological agents  
 IT Blood  
 Urine  
     (analysis, determination of vitamin B complex)  
 IT Carcinogenic substances  
     Pharmaceuticals  
         (cytotoxicity determination of, protozoa in)  
 IT Tetrahymena pyriformis  
     (in analysis for vitamins and cytotoxicity of carcinogens and pharmacol. agents)  
 IT Euglena gracilis  
 Ochromonas danica  
 Ochromonas malhamensis  
 Rhodopseudomonas palustris  
 Saccharomyces cerevisiae  
     (in analysis for vitamins and cytotoxicity of carcinogens and pharmacological agents)  
 IT Tissue, animal  
     (vitamin B complex in, determination of)  
 IT Cinnamonnitrile, p-[2-(diethylamino)ethoxy]- $\beta$ -ethyl- $\alpha$ -phenyl-, hydrochloride, trans-  
 IT Coccochloris elabens  
     (in analysis for vitamins and cytotoxicity of carcinogens and pharmacological agents)  
 IT Cinnamonnitrile, p-chloro- $\alpha$ -[p-[2-(diethylamino)ethoxy]phenyl]- $\beta$ -ethyl-, hydrochloride, trans-  
     (protozoa inhibition by)  
 IT 58-85-5, Biotin 59-43-8, Thiamine 59-67-6, Nicotinic acid 65-23-6, Pyridoxol 68-19-9, Vitamin B12 79-83-4, Pantothenic acid 12001-76-2, Vitamin B complex  
     (determination of, protozoa in)  
 IT 73-22-3, Tryptophan  
     (in protozoa response to 4-nitroquinoline 1-oxide)  
 IT 55-03-8, Thyroxine, sodium salt, L- 62-68-0, Valeric acid, 2,2-diphenyl-, 2-(diethylamino)ethyl ester, hydrochloride 65-49-6, Salicylic acid, 4-amino- 90-27-7, Butyric acid, 2-phenyl- 2278-46-8, 5 $\alpha$ -Pregn-3 $\beta$ -ol, 20 $\alpha$ -[(2-(dimethylamino)ethyl)amino]- 3039-68-7, Ethylamine, 2-[(2,2-diphenylpentyl)oxy]-N,N-dimethyl-, hydrochloride 3641-13-2, s-Triazole-3-carboxylic acid, 5-amino-3724-16-1, 3-Pyridineacetamide  
     (preparation of)  
 IT 148-07-2, Maleamic acid, N-[2,3-bis(p-chlorophenyl)-1-methylpropyl]-,  $\alpha$ -( $\pm$ )- 637-07-0, Propionic acid, 2-(p-chlorophenoxy)-2-methyl-, ethyl ester 27774-13-6, Vanadyl sulfate, VOSO4  
     (protozoa inhibition by)  
 IT 56-57-5, Quinoline, 4-nitro-, 1-oxide  
     (protozoa inhibition by, L-tryptophan as antagonist of)  
 IT 78-41-1, Ethanol, 2-(p-chlorophenyl)-1-[p-[2-(diethylamino)ethoxy]phenyl]-1-p-tolyl-  
     (protozoan inhibition by)  
 IT 61-82-5, s-Triazole, 3-amino- 6642-32-6, Urea, (5-phenyl-s-triazol-3-yl)-  
     (Ochromonas danica inhibition by)  
 ACCESSION NUMBER: 1966:29146 HCAPLUS  
 DOCUMENT NUMBER: 64:29146  
 ORIGINAL REFERENCE NO.: 64:5437c-g  
 TITLE: Protozoan assays for vitamins, and cytotoxicity of carcinogens, and pharmacological agents  
 AUTHOR(S): Aaronson, A.; Baker, H.; Bensky, B.; Frank, O.; Zahalsky, A. C.  
 CORPORATE SOURCE: Roosevelt Hosp., New York, NY  
 SOURCE: Develop. Ind. Microbiol. (1965), Volume Date

1964, 6, 48-58

DOCUMENT TYPE:

Journal

LANGUAGE:

English

ABSTRACT:

Protozoans were used for the assay of B vitamins in biol. samples of serum, urine, and tissues. The sensitivities of assays of thiamine, and biotin by using *Ochromonas danica* were, resp., 100 and 3 picograms/ml. The sensitivity limits of assays by using *Tetrahymena pyriformis* for nicotinic acid, vitamin B6, and pantothenic acid were 3 nanograms, 100 picograms, and 5 nanograms/ml., resp. *O. malhamensis* assayed vitamin B12 at a concentration of 1 picogram. *T. pyriformis*, and *O. malhamensis* were more specific for the several forms of nicotinic acid and vitamin B12. Of 19 different 1,2,4-triazoles tested against *O. danica*, the most active compound was 3-amino-1,2,4-triazole, followed by 3-carboxy-5-amino-1,2,4-triazole, and 3-amino-carboxamino-5-phenyl-1,2,4-triazole, which were, resp., 2-, and 4-fold less inhibitory. Several metabolic sites of aminotriazole inhibition of *O. danica* were located. The carcinogen, 4-nitro-quinoline-N-oxide (I), 1 mg. %, completely inhibited the growth of *O. danica*, and *Euglena gracilis*, and the inhibition was annulled by L-tryptophan, .apprx.4 mg. %, in both species. The tryptophan-transport system in protozoans was affected during I inhibition. The protozoan multiplication was inhibited to different degrees by hypocholesterolemic agents such as VOSO4, p-aminosalicyclic acid,  $\alpha$ -phenylbutyric acid, Na L-thyroxinate, benzmalecene, triparanol (MER-29), 22,25-diazocholestanol,  $\beta$ -diethylaminoethyldiphenylpropylacetate (SKF-525A), 2,2 diphenyl-1- $\beta$ -dimethylaminoethoxy pentane (SKF-3301A), trans-3-[p-diethylaminoethoxy]phenyl]-2-phenyl-2-pentenenitrile (P-3013), and trans-3-(p-chlorophenyl)-2-(p-diethylaminoethoxy)-phenyl-2-pentenenitrile (P-3429). Oleic acid overcame inhibition of *O. danica* by a variety of above-named compds. with different inhibitory sites on mammalian sterol biosynthesis. The major sites of action of several hypocholesterolemic agents on sterol-synthesizing microorganisms, *Saccharomyces cerevisiae*, *E. gracilis*, and *O. danica*, and in nonsterol-synthesizing microorganisms, *T. pyriformis*, *Rhodopseudomonas palustris*, and *Coccochloris elabens*, was apparently on the metabolism of unsatd. fatty acids rather than sterol metabolism. Unsatd. but not saturated fatty acids annulled the inhibition of *Ochromonas* respiration induced by several hypocholesterolemic agents.

L18 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

CC 1 (Pharmacodynamics)

TI Y and Z, two hepatic cytoplasmic organic anion-binding proteins. Effect of drugs, chemicals, hormones, and cholestasis

ST protein organic anion binding; drugs anion binding protein; hormones anion binding protein; Y anion binding protein; Z anion binding protein

IT Anions

(absorption of organic, by liver, pharmaceuticals effect on)

IT Pituitary gland

Thyroid gland

Hormones

RL: BIOL (Biological study)

(in organic anion metabolism by liver, protein binding in relation to)

IT Proteins

RL: BIOL (Biological study)

(of liver, in organic anion transport, pharmaceuticals effect on)

IT Biological transport

(of organic anions, by liver, pharmaceuticals effect on)

IT Liver, metabolism

(of organic anions, transport and binding by proteins in, pharmaceuticals effect on)

IT 50-29-3, biological studies 50-32-8 51-48-9, biological studies

56-49-5 57-30-7 57-63-6 60-57-1 64-17-5, biological studies

299-78-5

RL: BIOL (Biological study)

(organic anion metabolism by liver response to, protein binding in

relation to)

ACCESSION NUMBER: 1972:30614 HCPLUS  
 DOCUMENT NUMBER: 76:30614  
 TITLE: Y and Z, two hepatic cytoplasmic organic anion-binding proteins. Effect of drugs, chemicals, hormones, and cholestasis  
 AUTHOR(S): Reyes, Humberto; Levi, A. Jonathan; Gatmaitan, Zenaida; Arias, Irwin M.  
 CORPORATE SOURCE: Dep. Med., Albert Einstein Coll. Med., Bronx, NY, USA  
 SOURCE: Journal of Clinical Investigation (1971), 50(11), 2242-52  
 CODEN: JCINAO; ISSN: 0021-9738  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ABSTRACT:

The hepatic content of the 2 cytoplasmic proteins, Y and Z, that bind various organic anions and the organic anion transfer from plasma to liver (as determined by initial plasma disappearance rate of sulfobromophthalein [71-67-0]) increased in rats after 1-2 week administration of phenobarbital (I) [50-06-6] (80 mg/kg, s.c.), allylisopropylacetamide [299-78-5] (300 mg/kg s.c.), dieldrin [60-57-1] (20 mg/kg, s.c.), DDT [50-29-3] (20 mg/kg, s.c.), 3-methylcholanthrene [56-49-5] (10 mg/kg, s.c.) and benzpyrene [50-32-8] (10 mg/kg, s.c.).  
 \*\*\*Ethanol\*\*\* [64-17-5] feeding (36% of the caloric intake) for 5.5 weeks had no effect on hepatic content of Y or Z or on plasma-to-liver organic anion transfer. Hypophysectomy and thyroideectomy increased hepatic Y content but decreased organic anion transfer in rats. The increased Y content observed in rats with congenital pituitary insufficiency was returned to normal levels by \*\*\*thyroxine\*\*\* [51-48-9] administration. I caused a further increase in hepatic Y content when given to hormone deficient rats, suggesting different mechanisms for changes in Y by drug administration and hormone deprivation.  
 \*\*\*Thyroxine\*\*\* [51-48-9], testosterone [58-22-0], or hydrocortisone [50-23-7] had no effect on hepatic Y content or organic anion transfer in normal rats. Cholestasis produced by either ethinyl estradiol [57-63-6] or by biliary obstruction decreased hepatic Y and Z content and organic anion transfer.

L18 ANSWER 9 OF 9 HCPLUS COPYRIGHT 2006 ACS on STN

INCL 167065000  
 CC 30 (Pharmaceuticals)  
 TI Reduction of plasma cholesterol  
 IT Blood plasma  
     (cholesterol in, preps. for lowering of)  
 IT Casein, Caseinogen  
     (iodinated, in cholesterol lowering in blood plasma)  
 IT 101-40-6, Cyclohexaneethylamine, N, $\alpha$ -dimethyl- 543-82-8,  
     Hexylamine, 1,5-dimethyl-  
     (as cough inhibitor)  
 IT 57-88-5, Cholesterol  
     (in blood plasma, pharmaceutical for lowering of)  
 IT 78-41-1, Ethanol, 2-(p-chlorophenyl)-1-[p-[2-(diethylamino)ethoxy]phenyl]-1-p-tolyl-  
     (in cholesterol in blood plasma lowering)  
 IT 51-48-9, Thyroxine 434-13-9, 5 $\beta$ -Cholanic acid,  
     3 $\alpha$ -hydroxy-  
     (in cholesterol lowering in blood plasma)  
 ACCESSION NUMBER: 1965:2573 HCPLUS  
 DOCUMENT NUMBER: 62:2573  
 ORIGINAL REFERENCE NO.: 62:408c-d  
 TITLE: Reduction of plasma cholesterol  
 INVENTOR(S): Bosshardt, David K.; Howe, Eugene E.; Huff, Jesse W.  
 PATENT ASSIGNEE(S): Merck & Co., Inc.  
 SOURCE: 3 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3153615		19641020	US 1962-235836	19621106 <--

## ABSTRACT:

The cholesterol content of mammalian plasma is lowered by incorporating in the diet 0.05-1.0% by weight lithocholic acid in conjunction either with a thyroid-active substance, such as iodinated casein or thyroxin, or with an inhibitor of cholesterol synthesis such as Triparanol [1-[p-( $\beta$ -diethylaminoethoxy)phenyl]1-(p-tolyl)-2-(p-chlorophenyl)ethanol].

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	50.07	247.68
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-8.25	-13.50

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	4.41	252.09
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-13.50

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